The following full text is a preprint version which may differ from the publisher's version.

For additional information about this publication click this link.
http://hdl.handle.net/2066/84349

Please be advised that this information was generated on 2017-12-20 and may be subject to change.
Improving posterior marginal approximations in latent Gaussian models

Botond Cseke
Radboud University Nijmegen, Institute for Computing and Information Sciences
Nijmegen, The Netherlands
{b.cseke,t.heskes}@science.ru.nl

Tom Heskes
Radboud University Nijmegen, Institute for Computing and Information Sciences
Nijmegen, The Netherlands
{b.cseke,t.heskes}@science.ru.nl

Abstract

We consider the problem of correcting the posterior marginal approximations computed by expectation propagation and Laplace approximation in latent Gaussian models and propose correction methods that are similar in spirit to the Laplace approximation of Tierney and Kadane (1986). We show that in the case of sparse Gaussian models, the computational complexity of expectation propagation can be made comparable to that of the Laplace approximation by using a parallel updating scheme. In some cases, expectation propagation gives excellent estimates, where the Laplace approximation fails. Inspired by bounds on the marginal corrections, we arrive at factorized approximations, which can be applied on top of both expectation propagation and Laplace. These give nearly indistinguishable results from the non-factorized approximations in a fraction of the time.

1 Introduction

Following Rue et al. (2009), we consider the problem of computing marginal probabilities over single variables in (sparse) latent Gaussian models. Probabilistic models with latent Gaussian variables are of interest in many areas of statistics, such as spatial data analysis (Rue and Held, 2005), and machine learning, such as Gaussian process models (e.g. Kuss and Rasmussen, 2005). The general setting considered in Rue et al. (2009) as well as in this paper is as follows. The prior distribution over the latent variables is a Gaussian random field with a sparse precision (inverse covariance) matrix and the likelihood factorizes into a product of terms depending on just a single latent variable. Both the prior and the likelihood may depend on a small set of hyper-parameters (say at most 6 in total). We are interested in the posterior marginal probabilities over single variables given all observations.

Rue et al. (2009) propose an integrated nested Laplace approximation to approximate these posterior marginal distributions. Their procedure consists of three steps. 1) Approximate the posterior of the hyper-parameters given the data and use this to determine a grid of hyper-parameter values. 2) Approximate the posterior marginal distributions given the data and the hyper-parameters values on the grid. 3) Numerically integrate the product of the two approximations to obtain the posterior marginals of interest. The crucial contribution is the improved marginal posterior approximation in step 2), based on the approach of Tierney and Kadane (1986), that goes beyond the Gaussian approximation and takes into account higher order characteristics of (all) likelihood terms. Comparing their approach with Monte Carlo sampling techniques on several high-dimensional models, they show that their procedure is remarkably fast and accurate.

The main objective of the current paper is to see whether we can improve upon the approach of Rue et al. (2009). Expectation propagation, a method for approximate inference developed and studied mainly in the machine learning community, is then an obvious candidate. It is well-known to yield approximations that are more accurate than the Laplace approximation (e.g. Minka, 2001; Kuss and Rasmussen, 2005). Furthermore, expectation propagation can still be applied in cases where the Laplace approximation is doomed to fail, e.g., when the log-posterior is not twice-differentiable (Seeger, 2008). The typical price to be paid is that of higher computational complexity. However, we will see that, using a parallel instead of a sequential updating scheme, expectation propa-
Improving posterior marginal approximations in latent Gaussian models

In the context of sparse Gaussian models with many latent variables, the Laplace approximation is at most a (relatively small) constant factor slower than the Laplace approximation in applications. Moreover, along the way we will arrive at further approximations (both for expectation propagation and the Laplace approximation) that yield an order of magnitude speed-up, with hardly any degradation of performance.

Section 1.1 specifies the model and introduces notation, Section 2 introduces and compares several methods for correcting marginals given a fixed setting of the hyper-parameters, Section 3 discusses the computational complexity of these methods when applied to sparse models, and Section 4 treats integration over hyper-parameters.

1.1 Sparse latent Gaussian models

In this section we introduce notation and define the models under consideration. Let \( p(y|x, \theta) \) be the conditional probability of the observations \( y = (y_1, \ldots, y_n)^T \) given the latent variables \( x = (x_1, \ldots, x_n)^T \) and the hyper-parameters \( \theta \). We assume that this likelihood factorizes over the latent variables:

\[
P(y|x, \theta) = \prod_{i=1}^{n} p(y_i|x_i, \theta).
\]

The prior \( p(x|\theta) \) over the latent variables is Gaussian, e.g., a Gaussian process or a so-called thin plate spline mimicking prior on a two-dimensional grid (Rue et al., 2009). We call such a model “sparse”, when the precision (inverse covariance) matrix of the Gaussian prior is sparse. Furthermore, we assume that the number of hyper-parameters \( \theta \) is relatively small, say at most 6. We will omit \( p(y|x, \theta) \)'s and \( p(x|\theta) \)'s dependence on \( \theta \) whenever it is not relevant, use \( p_0(x) \) as an alias of the prior \( p(x|\theta) \), and \( q(x) \) for an approximating Gaussian distribution.

2 Posterior marginals conditioned upon the hyper-parameters

2.1 Global approximations

In this section we will focus on approximating posterior marginal distributions given a fixed setting of the hyper-parameters \( \theta \), which is omitted from the notation. That is, our goal is to approximate

\[
p(x_i|y) = \frac{1}{Z} t_i(x_i) \int dx_j p_0(x) \prod_{j \neq i} t_j(x_j),
\]

where we used shorthand notation \( t_i(x_i) \equiv p(y_i|x_i) \) and with normalization constant

\[
Z = \int dx \ p_0(x) \prod_{i} t_i(x_i),
\]

which in fact corresponds to the “evidence” \( p(y|\theta) \) that we need in order to compute the posterior \( p(\theta|y) \). In the following we will describe several approximation procedures. Discussion of the corresponding computational complexities is postponed until Section 3.

As a first step, we construct a global Gaussian approximation \( q(x) \) of \( p(x) \), e.g., through expectation propagation (EP) or using Laplace’s method. The approximation obtained through EP is of the form

\[
q(x) = \frac{1}{Z_q} p_0(x) \prod_{i} \tilde{t}_i(x_i),
\]

where \( \tilde{t}_i(x_i) \) are so-called Gaussian term proxies and \( Z_q \) ensures proper normalization. A Gaussian term proxy has the form of a Gaussian, but need not be normalized nor normalizable, i.e., may have a negative precision. Expectation propagation iteratively improves the term proxies one by one. When updating the \( i \)th term proxy given all other term proxies, the new term proxy \( \tilde{t}_i(x_i) \) is chosen such that

\[
\int dx_i \{1, x_i, x_i^2\} q^{(i)}(x_i) \tilde{t}_i(x_i) = \int dx_i \{1, x_i, x_i^2\} q^{(i)}(x_i) t_i(x_i),
\]

with the “cavity” distribution, the Gaussian approximation with the \( i \)th term proxy left out,

\[
q^{(i)}(x) \propto p_0(x) \prod_{j \neq i} \tilde{t}_j(x_j).
\]

That is, we choose the new term proxy \( \tilde{t}_i(x_i) \) such that the moments (up to second order) of “cavity times term proxy” equal those of “cavity times actual term”. The solution of this “moment matching” operation is typically found through numerical integration. We refer to (Minka, 2005; Kuss and Rasmussen, 2005; Seeger, 2008) for more information on (how to use) EP for approximate inference in Gaussian processes and other models.

The global Gaussian approximation based on Laplace’s method is obtained by first finding the mode \( m = \arg \max_x \log p(x, y) \), and then setting the covariance matrix to the negative inverse of the Hessian, \( H(x) = \frac{\partial^2}{\partial x \partial x^T} \log p(x, y) \), evaluated at \( m \).

Below we will describe a parallel updating scheme which, for sparse models, is a lot faster than the standard sequential scheme.
It is easy to see that this Hessian amounts to the (sparse) precision matrix from the prior $p_0(x)$ plus diagonal terms corresponding to second derivatives of the log $t_i(x_i)$ terms. Consequently, also the Gaussian approximation resulting from Laplace's method can be written in the form (3) and, if desired, the corresponding term proxies can be used for initialization of the EP algorithm. The marginal $q(x_i)$ of the global Gaussian approximation (3) can be considered our lowest order approximation of the posterior marginal distribution of interest. We will write $\tilde{p}_i^\text{EP}(x_i)$ for the Gaussian marginal following from the EP approximation and $\tilde{p}_i^\text{LA}(x_i)$ for the marginal following from Laplace's method. In the following, we will discuss how to improve upon these global approximations.

2.2 Marginal corrections

Given a global Gaussian approximation $q(x)$ of the form (3) with corresponding term proxies, we can rewrite (1) as

$$p(x_i|y) = \frac{Z_q}{t_i(x_i)} \int dx_{\setminus i} q(x) \prod_{j \neq i} t_j(x_j) = \frac{Z_q}{t_i(x_i)} q(x_i) \prod_{j \neq i} t_j(x_j)$$

$$= \frac{Z_q}{t_i(x_i)} \epsilon_i(x_i) \int dx_{\setminus i} q(x_{\setminus i}|x_i) \prod_{j \neq i} t_j(x_j)$$

where we defined $\epsilon_i(x_i) = t_i(x_i)/t_i(x_i)$.

Equation (5), which is still exact, shows that there are two corrections to the Gaussian approximation $q(x_i)$: one direct, local correction through $\epsilon_i(x_i)$ and one more indirect correction through the (weighted integral over) $\epsilon_j(x_j)$’s for $j \neq i$. The direct, local correction comes without additional cost and suggests a second approximation,

$$p(x_i|y) \approx \epsilon_i(x_i) q(x_i)$$

which will be denoted $\tilde{p}_i^\text{EP-L}(x_i)$ and $\tilde{p}_i^\text{LA-L}(x_i)$ for the approximations following the global EP and Laplace approximation, respectively. The approximation $\tilde{p}_i^\text{EP-L}(x_i)$ is the marginal of EP’s “tilted” distribution $q_i(x) \propto t_i(x_i) q_i(x)$ (e.g. Minka, 2001; Opper et al., 2009).

To improve upon this approximation, we somehow have to get a handle on the indirect correction

$$c_i(x_i) \equiv \int dx_{\setminus i} q(x_{\setminus i}|x_i) \prod_{j \neq i} \epsilon_j(x_j)$$

The observation here is that, for each $x_i$, we are in fact back to the form (2): we have to estimate the normalization constant of a sparse latent Gaussian model, where $q(x_{\setminus i}|x_i)$ now plays the role of a sparse $(n-1)$-dimensional Gaussian prior and the $\epsilon_j(x_j)$ are terms depending on a single variable. The idea is to choose a grid of $x_i$ values, compute $c_i(x_i)$ for each value of $x_i$ using our favorite method for computing normalization constants, and numerically interpolate between the resulting approximations. Running a complete procedure, be it EP or Laplace’s method, for each $x_i$ is often computationally too intensive and further approximations are needed to reduce the computational burden.

2.2.1 EP corrections

Let us write $\tilde{\epsilon}_j(x_j; x_i)$ for the term proxy of $\epsilon_j(x_j)$ in the context of approximating $c_i(x_i)$. A full run of EP for each $x_i$ may be too expensive, so instead we propose to make just one parallel step. Since the term proxies of the global EP approximation are tuned to make $\tilde{t}_j(x_j)$ close to $t_j(x_j)$, it makes sense to initialize $\tilde{\epsilon}_j(x_j; x_i)$ to 1. Following the same procedure as in (4), computing the new term proxy for term $j$ then amounts to choosing $\tilde{\epsilon}_j(x_j; x_i)$ such that

$$\int dx_{\setminus j} \{1, x_j, x_j^2\} q(x_j|x_i) \tilde{\epsilon}_j(x_j; x_i) = \int dx_{\setminus j} \{1, x_j, x_j^2\} q(x_j|x_i) \epsilon_j(x_j)$$

Replacing the terms $\epsilon_j(x_j)$ in (6) by their term proxies $\tilde{\epsilon}_j(x_j; x_i)$ yields an estimate for $c_i(x_i)$. The corresponding approximation

$$p(x_i|y) \approx \epsilon_i(x_i) q(x_i) \prod_{j \neq i} \tilde{\epsilon}_j(x_j; x_i)$$

is referred to as $\tilde{p}_i^\text{EP-1STEP}(x_i)$.

2.2.2 Laplace corrections

In our setting, the approximation proposed by Rue et al. (2009) can be understood as follows. In principle, one could, following Tierney and Kadane (1986), run a Laplace approximation on

$$f(x_{\setminus i}; x_i) = q(x_{\setminus i}|x_i) \epsilon_j(x_j)$$

To do this, one would need to compute, for each value of $x_i$, the mode of $f(x_{\setminus i}; x_i)$ as well as (the determinant of minus) the Hessian of log $f(x_{\setminus i}; x_i)$, evaluated at this mode. We will refer to the corresponding approximation as $\tilde{p}_i^\text{LA-TK}(x_i)$. Because finding the optimum of $f(x_{\setminus i}; x_i)$ is computationally rather expensive, Rue et al. (2009) propose to replace the mode of $f(x_{\setminus i}; x_i)$ by the mode of $q(x_{\setminus i}|x_i)$, i.e., the conditional mean of the Laplace approximation, and to evaluate the Hessian at this conditional mean. The corresponding approximation, which we will refer to as $\tilde{p}_i^\text{LA-CM}(x_i)$,
Improving posterior marginal approximations in latent Gaussian models

Posterior marginal of the component $x_1$

Figure 1: Various marginal corrections for a probit model with $t_i(x_i) = \Phi(4x_i)$ and identical variances and correlations in the prior $p_0$, using expectation propagation (top row) and Laplace-type approximations (bottom row). The panels show the corrections for a three-dimensional model with prior variances and correlations $(v, c) = (1, 0.25)$ (left), $(v, c) = (4, 0.9)$ (middle) and for a 32-dimensional model $(v, c) = (4, 0.95)$ (right).

is of the form (8), where now $\tilde{\epsilon}_j(x_j; x_i)$ follows from a second-order Taylor expansion of $\log \epsilon_j(x_j)$ around the mode (and thus mean) of $q(x_j | x_i)$.

In order to further reduce computational effort, Rue et al. (2009) suggest additional approximations that, because they can only be expected to reduce the accuracy of the final approximation, will not be considered in our experiments in Sections 2.3 and 4.

2.2.3 Bounds and factorized approximations

As we will discuss below, the computational bottleneck in the above procedures for approximating the correction $c_i(x_i)$ is not computing appropriate approximations of the terms $\epsilon_j(x_j)$, either through EP or using Laplace’s method, but instead computing the normalization of the resulting Gaussian form which boils down to the computation of the determinant of a sparse matrix. Here we propose a simplification, which we motivate through its connection to bounds on the marginal correction $c_i(x_i)$.

Using Jensen’s inequality, we obtain the lower bound

$$c_i(x_i) \geq \exp \left[ \sum_{j \neq i} \int dx_j q(x_j | x_i) \log \epsilon_j(x_j) \right] = c_i^\ell(x_i).$$

Following Minka (2005), we can also get an upper bound:

$$c_i(x_i) \leq \prod_{j \neq i} \left[ \int dx_j q(x_j | x_i) \epsilon_j(x_j)^{n-1} \right]^{1/(n-1)} = c_i^u(x_i).$$

This upper bound will in many cases be useless because the integral does not exist. The lower bound, which corresponds to a mean-field-type approximation, does not have this problem, but may still be somewhat conservative. We therefore propose the general family of approximations

$$c_i^{(\alpha)}(x_i) = \prod_{j \neq i} \left[ \int dx_j q(x_j | x_i) \epsilon_j(x_j) \right]^{\alpha/(n-1)}.

It is easy to show that

$$c_i^\ell(x_i) \leq c_i^{(\alpha)}(x_i) \leq c_i^u(x_i) \quad 0 \leq \alpha \leq n-1,$$

where $\alpha = 0$ is interpreted as the limit $\alpha \to 0$. The choice $\alpha = 1$ makes the most sense: it gives exact results for $n = 2$ as well as when all $x_j$’s (indeed) happen to be conditionally independent given $x_i$. We refer to the corresponding approximation as $p_i^{\text{EP-FACT}}(x_i)$.

Using (7), it is easy to see that $p_i^{\text{EP-FACT}}(x_i)$ corresponds to $p_i^{\text{EP-1STEP}}(x_i)$ if in (8) we would replace $q(x_i | x_i)$ by the factorization $\prod_{j \neq i} q(x_j | x_i)$, i.e., as if the variables $x_j$ in the global Gaussian approximation are conditionally independent given $x_i$. The same replacement in the Laplace approximation yields the approximation referred to as $p_i^{\text{LA-FACT}}(x_i)$.
2.2.4 Taylor expansions

To make the connection to the earlier work in (Opper et al., 2009), we expand the exact $c_i(x_i)$ of (6) in $\epsilon_j(x_j) - 1$ for all $j \neq i$. Keeping only lowest order terms, we obtain

$$c_i(x_i) \approx 1 + \sum_{j \neq i} \int dx_j q_j(x_j | x_i) [\epsilon_j(x_j) - 1] \equiv c_i^{\text{TAYLOR}}(x_i),$$

which coincides with the Taylor expansion of $c_i^{(\alpha)}(x_i)$ of (9) for any $\alpha$. An obvious approximation would be

$$p_i(x_i) \approx q_i(x_i) \epsilon_i(x_i) c_i^{\text{TAYLOR}}(x_i). \quad (10)$$

The approximation proposed in (Opper et al., 2009) goes one step further by Taylor expanding not only $\epsilon_j(x_j)$ for $j \neq i$, but also $c_i(x_i)$ up to the same order, which boils down to

$$p_i(x_i) \approx q_i(x_i) [\epsilon_i(x_i) + c_i^{\text{TAYLOR}}(x_i) - 1] \equiv p_i^{\text{EP-OPW}}(x_i). \quad (11)$$

Computing $p_i^{\text{EP-OPW}}(x_i)$ is as expensive as computing $p_i^{\text{EP-FACT}}(x_i)$. Where $p_i^{\text{EP-OPW}}(x_i)$ can yield negative probabilities, $p_i^{\text{EP-FACT}}(x_i)$ is nonnegative by construction. Furthermore, $p_i^{\text{EP-FACT}}(x_i)$ appears to be more accurate (see below), if only because it prevents the unnecessary step from (10) to (11).

2.3 Comparisons on toy models

To illustrate the correction methods, we take a probit model with $t(x_i) = \Phi(4x_i)$, with $\Phi$ the Gaussian cumulative density function, and a zero-mean prior $p_0$ with covariance matrix $Q^{-1} = \nu((1 - c)I + c11^T)$. The left and middle panels in Figure 1 show the marginal corrections of the first component for a three-dimensional model with $(\nu, c) = (1, 0.25)$ and $(\nu, c) = (4, 0.95)$, respectively. The bars, in this and all other figures, correspond to a large number of Monte Carlo samples, either obtained through Gibbs or Metropolis sampling, and are supposed to represent the gold standard.

The local correction $p_i^{\text{EP-L}}$ yields sufficiently accurate approximations when the correlations are weak (left-top), but is clearly insufficient when they are strong (middle-top). The corrections $p_i^{\text{EP-1STEP}}$ and $p_i^{\text{EP-FACT}}$ yield accurate estimates and are almost indistinguishable even for strong prior correlations. Only when we increase the number of dimensions (here from 3 to 32) and with strong correlations $(\nu, c) = (4, 0.95)$, we can see small differences (right-top). As we can see on Figure 1, $p_i^{\text{EP-OPW}}$ does slightly worse than $p_i^{\text{EP-FACT}}$ and can indeed go negative.

It is known that the Laplace-type approximations does not perform well on this model (e.g. Kuss and Rasmussen, 2005). The approximations tend to be acceptable for weak correlations (bottom-left), with $p_i^{\text{LA-CM}}$ and $p_i^{\text{LA-FACT}}$ clearly outperforming $p_i^{\text{LA}}$ and $p_i^{\text{LA-L}}$, but are far off when the correlations are strong (bottom-middle). The Laplace corrections suffer from essentially the same problems as the global Gaussian approximation based on Laplace’s method: the mode and the inverse Hessian badly represent the mean and the covariance and fail to sufficiently improve it.

Expectation propagation can still be applied when the Laplace approximation is doomed to fail. An example is Bayesian linear regression with a double-exponential prior (Seeger, 2008). Direct application of the Laplace approximation makes no sense, because there is no local curvature information available that properly represents the behavior of the function $|x|$. Figure 2 describes a toy model with the same characteristics. It can be seen that the lowest order (Gaussian) EP approximation gets the mass right, but not the shape. Local corrections already help a lot, and both factorized and one-step EP corrections are practically indistinguishable from the sampling results.

We compared the various methods on several other toy models (not shown due to lack of space), leading to similar observations. It is relatively easy to come
up with models on which (all) Laplace-type approxi-
mations fail and expectation propagation, in particu-
lar EP-1STEP and EP-FACT are still fine. It is a lot
harder to find cases where the factorized approxima-
tions EP-FACT and LA-FACT give quite different results
than the non-factorized and computationally more ex-
pensive EP-1STEP and LA-CM: for this we really need
to go to high dimensions and strong correlations.

3 Inference in sparse models

In this section we review the computational complex-
ities of the Laplace approximation and expectation
propagation when applied to sparse Gaussian models,
i.e., models for which the n-dimensional precision ma-
trix $Q$ of the Gaussian prior is sparse. Is expectation
propagation indeed orders of magnitude slower as sug-
gested in (Rue et al., 2009)?

3.1 Global approximations

The computational complexity for the Gaussian ap-
proximation based on both Laplace’s method and ex-
pectation propagation is dominated by several opera-
tions. 1) Computing the Cholesky factor, say $L$ of a
matrix $Q$, e.g., corresponding to the posterior approxi-
mation $\tilde{p}^A$ or $\tilde{p}^A$, with the same sparsity structure as
the prior precision matrix $Q$. The computational com-
plexity, denoted $c_{\text{chol}}$, in the worst case scales with $n^3$,
but typically with $\text{nnzeros}(Q)^2/n$, with $\text{nnzeros}(Q)$
the number of non-zeros in the precision matrix $Q$.
2) Computing the diagonal elements of the inverse of
$Q$. For sparse matrices, these can be computed effi-
ciently by solving the Takahashi equations (e.g. Eris-
man and Tinney, 1975; Rue et al., 2009), which take
the Cholesky factor $L$ as input. The computational com-
plexity, denoted $c_{\text{taka}}$, in the worst case scales with $n^3$,
but typically with $\text{nnzeros}(L)^2/n$. In prac-
tice, we experienced that it is significantly more ex-
pensive than the Cholesky factorization, possibly due to
our implementation. 3) Solving a triangular system of
the form $La = b$, with corresponding computational com-
plexity $c_{\text{tria}} \propto \text{nnzeros}(L)$.

To keep the number of non-zeros in the Cholesky fac-
tor to a minimum, we apply the approximate minimum
degree reordering algorithm (Amestoy et al., 1996),
which is claimed to have the best average per-
formance (Ingram, 2006). Since the sparsity structure is
fixed, this reordering algorithm has to be run only
once, prior to running any other algorithm.

Laplace’s method. The maximum a-posteriori so-
lution required for Laplace’s method can be found,
for example, through a Newton method. Each New-
ton step requires one Cholesky factorization and the solution of two triangular systems. To arrive at the
lowest-order marginals $\tilde{p}^A_i$ for all nodes $i$, we need the
diagonal elements of the covariance matrix, which can
be computed by solving the Takahashi equations us-
ing the Cholesky factor from the last Newton step.
So, in total, computing the lowest order marginals
$\tilde{p}^A_i$ for all nodes $i$ using Laplace’s method scales with
$n_{\text{steps}} \times (c_{\text{chol}} + 2 \times c_{\text{tria}}) + c_{\text{taka}}$.

Expectation propagation. To update a term approx-
imation $\hat{t}_i(x_i)$ according to Equation (4), we com-
pute $q^{(i)}(x_i) \propto q(x_i)/\hat{t}_i(x_i)$ using the marginals $q(x_i)$
from the current global approximation $q(x)$ and re-
estimate the normalization constant and the first two
moments of $\hat{t}_i(x_i) q^{(i)}(x_i)$. In standard practice, term
approximations $\hat{t}_i$ are updated sequentially and all
marginal means and variances are recomputed using
rank one updates after term each update. Instead,
we adopt a parallel strategy, that is, we recompu-
te marginal means and variances only after we have up-
dated all term approximations $\hat{t}_i$, $i = 1, \ldots, n$.

A parallel EP step boils down to: 1) compute the
Cholesky factorization of the current precision ma-
trix, 2) solve two triangular systems to compute the
current posterior mean and solve the Takahashi equa-
tions to compute the diagonal elements of the covari-
cance matrix, and 3) if necessary, use univariate Gauss-
Hermite numerical quadrature with $n_{\text{quad}}$ nodes to
compute the quantities in Equation (4). This adds
up to a computational complexity that scales with
$n_{\text{steps}} \times (c_{\text{chol}} + 2 \times c_{\text{tria}} + c_{\text{taka}} + n \times n_{\text{quad}})$. After
convergence, EP yields the lowest order marginals $\tilde{p}^E_i$ for all nodes $i$.

Summarizing, because of the parallel scheme, we
use exactly the same computational tricks as with
Laplace’s method (Cholesky, Takahashi). Initializing
the term approximations in EP from the Laplace so-
lution and then doing a few EP steps to obtain better
estimates of the probability mass, makes EP just a
(small) constant factor slower than Laplace.

3.2 Marginal corrections

After running the global approximation, we are left
with some Gaussian $q(x)$ with known precision ma-
trix, a corresponding Cholesky factor and single-node
marginals $q(x_i)$. We now consider the complexity of
computing a corrected marginal through the various
methods for a single node $i$, using $n_{\text{grid}}$ grid points
(see the summary in Table 1). The local corrections $\tilde{p}^L_i$ and $\tilde{p}^E_i$ we get more or
less for free. All other correction methods require
the computation of the conditional densities \( q(x_j | x_i) \), which amounts to solving two sparse triangular systems and \((n - 1) \times n_{\text{grid}}\) evaluations. To arrive at the term approximations \( \tilde{c}(x_j; x_i) \), we need to compute second order derivatives for the Laplace approximation and numerical quadratures for EP, which is about \( n_{\text{quad}} \) times more expensive. For LA-FACT, EP-FACT, and EP-OPW, we then simply have to compute a product/sum of \( n \) normalization terms. For LA-TK, LA-CM and EP-1STEP, we need to compute the determinant of an \((n - 1)\)-dimensional sparse matrix, which costs a Cholesky factorization.

### 4 Inference of the hyper-parameters

Until now, we considered estimating single-node marginals conditioned upon the hyper-parameters. In this section, we consider the estimation of the posterior marginals that follow by integrating over the hyper-parameters. For this we need the posterior of the hyper-parameters given the observations, which is approximated by \( \tilde{p}(\theta | y) \propto p(y | \theta) p(\theta) \), where \( \tilde{p}(y | \theta) \) is the marginal likelihood approximation provided by Laplace’s method or expectation propagation.

The basic idea is to compute the posterior mode of \( \tilde{p}(\theta | y) \) as well as the Hessian at this mode (using finite differences), select a set of uniformly spaced grid points along the scaled eigenvectors of this Hessian, and use these to perform numerical quadrature using the rectangle rule. We implemented a slight modification of the method used by Rue et al. (2009), which selects the grid points more efficiently (details to be given in an expanded report).

**Example.** As an example for a sparse Gaussian model we implemented the stochastic volatility model presented in (Rue et al., 2009). The data set consists of 945 samples of the daily difference of the pound-dollar exchange rate from October 1st, 1981, to June 28th, 1995. Similarly to Rue et al. (2009), we used the first 50 observations. The observations \( y_t \) given the latent variables \( \eta_t \) are taken to be distributed independently according to \( p(y_t | \eta_t) = N(y_t | 0, e^{\eta_t}) \).

The latent field \( \eta_t \) is assumed to be the sum \( \eta_t = f_t + \mu \) of a first-order auto-regressive Gaussian process \( p(f_t | f_{t-1}, \phi, \tau) = N(f_t | \phi f_{t-1}, 1/\tau) \), with \(|\phi| < 1\), and an additional Gaussian bias term \( p(\mu) = N(\mu | 0, 1) \).

The prior on the hyper-parameter \( \tau \) is taken to be \( p(\tau) = \Gamma(\tau | 1, 10) \) and a Gaussian prior \( N(0, 3) \) is taken over \( \phi = \log((1 + \phi)/(1 - \phi)) \).

The results are shown in Figure 3. The Laplace and EP approximation of the evidence are nearly indistinguishable (left), as are the posterior marginals of the hyper-parameters (middle-left). Here EP is about a factor 5 slower than Laplace. The posterior marginals of \( f_{50} \) and \( \mu \) obtained using the more involved methods (right half, bottom row) are practically indistinguishable from each other and the gold (sampling) standard. This is not the case for the cheaper variants LA, EP, and LA-L, but is the case for EP-L (right half, top row): apparently to obtain excellent posterior marginals on this model, there is no need for (computationally expensive) higher-order corrections, but it suffices to compute a single global EP approximation per hyper-parameter setting and correct this for the (non-Gaussian) local term.

### 5 Discussion

There are many options for further improvement, in particular w.r.t. efficiency. The ideas behind the simplified Laplace approximation of (Rue et al., 2009), which aims to prevent the expensive computation of a determinant for each \( x_i \), may well be applicable to expectation propagation. However, if this indeed dominates the computation times, the factorized approximation proposed in this paper may well be a better alternative. Incorporation of linear constraints on the latent variables, although not considered in this paper, should be relatively straightforward.

One of the main problems of expectation propagation is that it is not guaranteed to converge and may run into numerical problems. EP converged fine on the problems considered in this paper, but even when it does not, it can still be beneficial to start from the

<table>
<thead>
<tr>
<th>steps \ methods</th>
<th>LA-CM</th>
<th>LA-FACT</th>
<th>EP-1STEP</th>
<th>EP-FACT</th>
</tr>
</thead>
<tbody>
<tr>
<td>( q(x_j</td>
<td>x_i) )</td>
<td>( c_{\text{tria}} + n \times n_{\text{grid}} )</td>
<td>( c_{\text{tria}} + n \times n_{\text{grid}} )</td>
<td>( c_{\text{tria}} + n \times n_{\text{grid}} )</td>
</tr>
<tr>
<td>( \tilde{c}(x_j; x_i) )</td>
<td>( n \times n_{\text{grid}} )</td>
<td>( n \times n_{\text{grid}} )</td>
<td>( n \times n_{\text{grid}} \times n_{\text{quad}} )</td>
<td>( n \times n_{\text{grid}} \times n_{\text{quad}} )</td>
</tr>
<tr>
<td>Norm. or det.-s</td>
<td>( c_{\text{chol}} \times n_{\text{grid}} )</td>
<td>( n \times n_{\text{grid}} )</td>
<td>( c_{\text{chol}} \times n_{\text{grid}} )</td>
<td>( n \times n_{\text{grid}} )</td>
</tr>
</tbody>
</table>

Table 1: Computational complexities of the steps for computing an improved marginal approximation for a particular node \( i \) using the various methods. The frames highlight the complexities that typically dominate the computational time. \( c_{\text{tria}}, c_{\text{chol}}, \) and \( c_{\text{ala}} \) refer to solving a sparse triangular system, a Cholesky factorization, and Takahashi equations, respectively. \( n_{\text{grid}} \) refers to the number of grid points for \( x_i \) and \( n_{\text{quad}} \) to the number of quadrature points for \( x_j \).
Laplace solution and make just a few steps to get a better grip on the probability mass instead of relying on the mode and the curvature.

For models with weak correlations and smooth nonlinearities, any approximation method gives decent results. It may well be possible to come up with cases (strong correlations, hard nonlinearities), where any deterministic approximation method fails. Most interesting problems are somewhere in between, and for those we can hardly tell how advanced and computationally intensive approximation method we need. The heuristic suggested in (Rue et al., 2009), systematically increase the complexity and stop when you do not obtain further changes, appears risky. In particular when going from the factorized to the non-factorized approximations, it is often hard to see changes, but still both approximations can be pretty far off. It would be interesting to obtain a better theoretical understanding of the (asymptotic) approximation errors implied by the different approaches.

Acknowledgements

This research was supported by VICI grant 639.023.604 from the Netherlands Organization for Scientific Research (NWO). We would like to thank the anonymous reviewers and Havard Rue for valuable comments on an earlier version.

References


