Divide and conquer in ABC: Expectation-Progagation algorithms for likelihood-free inference

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ABC algorithms are notoriously expensive in computing time, as they require simulating many complete artificial datasets from the model. We advocate in this paper a “divide and conquer” approach to ABC, where we split the likelihood into \( n \) factors, and combine in some way \( n \) ‘local’ ABC approximations of each factor. This has two advantages: (a) such an approach is typically much faster than standard ABC; and (b) it makes it possible to use local summary statistics (i.e. summary statistics that depend only on the data-points that correspond to a single factor), rather than global summary statistics (that depend on the complete dataset). This greatly alleviates the bias introduced by summary statistics, and even removes it entirely in situations where local summary statistics are simply the identity function.

We focus on EP (Expectation-Propagation), a convenient and powerful way to combine \( n \) local approximations into a global approximation. Compared to the EP-ABC approach of Barthelmé and Chopin (2014), we present two variations; one based on the parallel EP algorithm of Cseke and Heskes (2011), which has the advantage of being implementable on a parallel architecture; and one version which bridges the gap between standard EP and parallel EP. We illustrate our approach with an expensive application of ABC, namely inference on spatial extremes.

1 Introduction

A standard ABC algorithm samples in some way from the pseudo-posterior:

\[
p_{\epsilon}^{\text{std}}(\theta|y^*) \propto p(\theta) \int p(y|\theta) I_{\{\|s(y) - s(y^*)\| \leq \epsilon\}} \, dy
\]

(1)

where \( p(y|\theta) \) denotes the likelihood of data \( y \in \mathcal{Y} \) given parameter \( \theta \in \Theta \), \( y^* \) is the actual data, \( s \) is some function of the data called a ‘summary statistic’, and \( \epsilon > 0 \). As discussed elsewhere in

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this book, there are various ways to sample from \( \{1\} \), e.g. rejection, MCMC (Marjoram et al. 2003), SMC (Sisson et al. 2007; Beaumont et al. 2009; Del Moral et al. 2012), etc., but they all require simulating a large number of complete datasets \( y^j \) from the likelihood \( p(y|\theta) \), for different values of \( \theta \). This is typically the bottleneck of the computation. Another drawback of standard ABC is the dependence on \( s \) as \( \epsilon \to 0 \), \( p_\epsilon^{\text{std}}(\theta|y^\star) \to p(\theta|s(y^\star)) \neq p(\theta|y^\star) \), the true posterior distribution, and there is no easy way to choose \( s \) such that \( p(\theta|s(y^\star)) \approx p(\theta|y^\star) \).

In this paper, we assume that the data may be decomposed into \( n \) “chunks”, \( y = (y_1, \ldots, y_n) \), and that the likelihood may be factorised accordingly:

\[
p(y|\theta) = \prod_{i=1}^n f_i(y_i|\theta)
\]

in such a way that it is possible to sample pseudo-data \( y_i \) from each factor \( f_i(y_i|\theta) \). The objective is to approximate the pseudo-posterior:

\[
p_\epsilon(\theta|y^\star) \propto p(\theta) \prod_{i=1}^n \left\{ \int f_i(y_i|\theta) I\left\{ \| s_i(y_i) - s_i(y_i^\star) \| \leq \epsilon \right\} dy_i \right\}
\]

where \( s_i \) is a “local” summary statistic, which depends only on \( y_i \). We expect the bias introduced by the \( n \) local summary statistics \( s_i \) to be much smaller than the bias introduced by the global summary statistic \( s \). In fact, there are practical cases where we may take \( s_i(y_i) = y_i \), removing this bias entirely.

Note that we do not restrict to models such that the chunks \( y_i \) are independent. In other words, we allow each factor \( f_i \) to implicitly depend on other data-points. For instance, we could have a Markov model, with \( f_i(y_i|\theta) = p(y_i|y_{i-1}, \theta) \), or even a model with a more complicated dependence structure, say \( f_i(y_i|\theta) = p(y_i|y_{1:i-1}, \theta) \). The main requirement, however, is that we are able to sample from each factor \( f_i(y_i|\theta) \). For instance, in the Markov case, this means we are able to sample from the model realisations of variable \( y_i \), conditional on \( y_{i-1} = y_{i-1}^\star \) and \( \theta \).

Alternatively, in cases where the likelihood does not admit a simple factorisation, one may replace it by some factorisable pseudo-likelihood; e.g. a marginal composite likelihood:

\[
p^{\text{MCL}}(y|\theta) = \prod_{i=1}^n p(y_i|\theta)
\]

where \( p(y_i|\theta) \) is the marginal density of variable \( y_i \). Then one would take \( f_i(y_i|\theta) = p(y_i|\theta) \) (assuming we are able to simulate from the marginal distribution of \( y_i \)). Conditional distributions may be used as well; see Varin et al. (2011) for a review of composite likelihoods. Of course, replacing the likelihood by some factorisable pseudo-likelihood adds an extra level of approximation, and one must determine in practice whether the computational benefits are worth the extra cost. Estimation based on composite likelihoods is generally consistent, but their use in a Bayesian setting results in posterior distributions that are overconfident (the variance is too small, as dependent data are effectively treated as independent observations).

Many authors have taken advantage of factorisations to speed up ABC. ABC strategies for hidden Markov models are discussed in Dean et al. (2014) and Yildirim et al. (2014); see the review of Jasra (2015). White et al. (2015) describe a method based on averages of pseudo-posteriors, which in the Gaussian case reduces to just doing one pass of parallel EP. Ruli et al. (2015) use composite likelihoods to define low-dimensional summary statistics.
We focus on Expectation Propagation (EP, Minka, 2001), a widely successful algorithm for variational inference. In Barthelmé and Chopin (2014), we showed how to adapt EP to a likelihood-free setting. Here we extend this work with a focus on a parallel variant of EP (Cseke and Heskes, 2011) that enables massive parallelisation of ABC inference. For textbook descriptions of EP, see e.g. Section 10.7 of Bishop (2006) or Section 13.8 of Gelman et al. (2014).

The chapter is organised as follows. Section 2 gives a general presentation of both sequential and parallel EP algorithms. Section 3 explains how to adapt these EP algorithms to ABC contexts. It discusses in particular some ways to speed up EP-ABC. Section 4 discusses how to apply EP-ABC to spatial extreme models. Section 5 concludes.

We use the following notations throughout: bold symbols refer to vectors or matrices, e.g. \( \mathbf{\theta}, \mathbf{\lambda}, \mathbf{\Sigma} \). For data-points, we use (bold) \( \mathbf{y} \) to denote complete datasets, and \( \mathbf{y}_i \) to denote data "chunks", although we do not necessarily assume the \( \mathbf{y}_i \)'s to be scalars. The letter \( p \) typically refers to probability densities relative to the model: \( p(\mathbf{\theta}) \) is the prior, \( p(\mathbf{y}_1 | \mathbf{\theta}) \) is the likelihood of the first data chunk, and so on. The transpose of matrix \( A \) is denoted \( A^t \).

2 EP algorithms

2.1 General presentation

Consider a posterior distribution \( \pi(\mathbf{\theta}) \) that may be decomposed into \( (n+1) \) factors:

\[
\pi(\mathbf{\theta}) \propto \prod_{i=0}^{n} l_i(\mathbf{\theta})
\]

where, say, \( l_0(\mathbf{\theta}) \) is the prior, and \( l_1, \ldots, l_n \) are \( n \) contributions to the likelihood. Expectation-Propagation (EP, Minka, 2001) approximates \( \pi \) by a similar decomposition

\[
q(\mathbf{\theta}) \propto \prod_{i=0}^{n} q_i(\mathbf{\theta})
\]

where each ‘site’ \( q_i \) is updated in turn, conditional on the other factors, in a spirit close to a coordinate-descent algorithm.

To simplify this rather general framework, one often assumes that the \( q_i \) belong to some exponential family of distributions \( Q \) (Seeger, 2005):

\[
q_i(\mathbf{\theta}) = \exp\left\{ \mathbf{\lambda}_i^t \mathbf{t}(\mathbf{\theta}) - \phi(\mathbf{\lambda}_i) \right\}
\]

where \( \mathbf{\lambda}_i \in \mathbb{R}^d \) is the natural parameter, \( \mathbf{t}(\mathbf{\theta}) \) is some function \( \Theta \to \mathbb{R}^d \), and \( \phi \) is known variously as the log-partition function or the cumulant function: \( \phi(\mathbf{\lambda}) = \log \left[ \int \exp \{ \mathbf{\lambda}^t \mathbf{t}(\mathbf{\theta}) \} d\mathbf{\theta} \right] \).

Working with exponential families is convenient for a number of reasons. In particular, the global approximation \( q \) is automatically in the same family, and with parameter \( \mathbf{\lambda} = \sum_{i=0}^{n} \mathbf{\lambda}_i \):

\[
q(\mathbf{\theta}) \propto \exp \left\{ \left( \sum_{i=0}^{n} \mathbf{\lambda}_i \right)^t \mathbf{t}(\mathbf{\theta}) \right\}.
\]

The next section gives additional properties of exponential families upon which EP relies. Then Section 2.2 explains how to perform a site update, that is, how to update \( \mathbf{\lambda}_i \), conditional on the \( \mathbf{\lambda}_j, j \neq i \), so as, informally, to make \( q \) progressively closer and closer to \( \pi \).
2.2 Properties of exponential families

Let $\text{KL}(\pi||q)$ be the Kullback-Leibler divergence of $q$ from $\pi$:

$$\text{KL}(\pi||q) = \int \pi(\theta) \log \frac{\pi(\theta)}{q(\theta)} \, d\theta.$$ 

For a generic member $q_\lambda(\theta) = \exp \left\{ \lambda^t t(\theta) - \phi(\lambda) \right\}$ of our exponential family $Q$, we have:

$$\frac{d}{d\lambda} \text{KL}(\pi||q_\lambda) = \frac{d}{d\lambda} \phi(\lambda) - \int \pi(\theta) t(\theta) \, d\theta \tag{2}$$

where the derivative of the partition function may be obtained as:

$$\frac{d}{d\lambda} \phi(\lambda) = \int t(\theta) \exp \left\{ \lambda^t t(\theta) - \phi(\lambda) \right\} \, d\theta = \mathbb{E}_\lambda \{t(\theta)\} \tag{3}.$$ 

Let $\eta = \eta(\lambda) = \mathbb{E}_\lambda \{t(\theta)\}$; $\eta$ is called the moment parameter, and there is a one-to-one correspondence between $\lambda$ and $\eta$: abusing notations, if $\eta = \eta(\lambda)$ then $\lambda = \lambda(\eta)$. One may interpret (2) as follows: finding the $q_\lambda$ closest to $\pi$ (in the Kullback-Leibler sense) amounts to perform moment matching, that is, to set $\lambda$ such that the expectation of $t(\theta)$ under $\pi$ and under $q_\lambda$ match.

To make this discussion more concrete, consider the Gaussian case:

$$q_\lambda(\theta) \propto \exp \left\{ -\frac{1}{2} \theta^t Q \theta + \phi(\lambda) \right\}, \quad \lambda = \left( r, -\frac{1}{2} Q \right), \quad t(\theta) = \left( \theta, \theta^t \right).$$

and the moment parameter is $\eta = (\mu, \Sigma + \mu \mu^t)$, with $\Sigma = Q^{-1}$, $\mu = Q^{-1} r$. (More precisely, $\theta^t Q \theta = \text{trace}(Q \theta \theta^t) = \text{vect}(Q)^t \text{vect}(\theta \theta^t)$, so the second component of $\lambda$ (respectively $t(\theta)$) should be $-(1/2) \text{vect}(Q)$ (resp. $\text{vect}(\theta \theta^t)$). But, for notational convenience, our derivations will be in terms of matrices $Q$ and $\theta \theta^t$, rather than their vectorised versions.)

In the Gaussian case, minimising $\text{KL}(\pi||q_\lambda)$ amounts to take $\lambda$ such that the corresponding moment parameter $(\mu, \Sigma + \mu \mu^t)$ is such that $\mu = \mathbb{E}_\pi \theta$, $\Sigma = \text{Var}_\pi \theta$. We will focus on the Gaussian case in this paper (i.e. EP computes iteratively a Gaussian approximation of $\pi$), but we go on with the more general description of EP in terms of exponential families, as this allows for more compact notations, and also because we believe that other approximations could be useful in the ABC context.

2.3 Site update

We now explain how to perform a site update for site $i$, that is, how to update given $\lambda_i$, assuming $(\lambda_j)_{j \neq i}$ is fixed. Consider the ‘hybrid’ distribution:

$$h(\theta) \propto q(\theta) \frac{l_i(\theta)}{q_i(\theta)} = l_i(\theta) \prod_{j \neq i} q_j(\theta) = l_i(\theta) \exp \left\{ \left( \sum_{j \neq i} \lambda_j \right)^t t(\theta) \right\}.$$
that is, \( h \) is obtained by replacing site \( q_i \) by the true factor \( l_i \) in the global approximation \( q \). The hybrid can be viewed as a “pseudo-posterior” distribution, formed of the product of a “pseudo-prior” \( q_i \) and a single likelihood site \( l_i \). The update of site \( i \) is performed by minimising \( \text{KL}(h\|q) \) with respect to \( \lambda_i \) (again, assuming the other \( \lambda_j, j \neq i \), are fixed). Informally, this may be interpreted as a local projection (in the Kullback-Leibler sense) of \( \pi \) to \( Q \).

Given the properties of exponential families laid out in the previous section, one sees that this site update amounts to setting \( \lambda_i \) so that
\[
\lambda_i = \sum_{j \neq i} \lambda_j \]
matches
\[
\mathbb{E}_h[t(\theta)] = \int t(\theta) l_i(\theta) \exp \left\{ (\lambda - \lambda_i) t(\theta) \right\} d\theta.
\]

\[4\]

**Algorithm 1** Generic site update in EP

**Function** SiteUpdate\((i, l_i, \lambda_i, \lambda)\):

1. Compute
\[
\lambda^\text{new}_i := \lambda \left( \mathbb{E}_h[t(\theta)] \right), \quad \lambda^\text{new} := \lambda^\text{new}_i - \lambda + \lambda_i
\]

where \( \eta \rightarrow \lambda(\eta) \) is the function that maps the moment parameters to the natural parameters (for the considered exponential family, see previous section) and

\[
\mathbb{E}_h[t(\theta)] = \frac{\int t(\theta) l_i(\theta) \exp \left\{ (\lambda - \lambda_i) t(\theta) \right\} d\theta}{\int l_i(\theta) \exp \left\{ (\lambda - \lambda_i) t(\theta) \right\} d\theta}.
\]

2. Return \( \lambda^\text{new}_i \), and optionally \( \lambda^\text{new} \) (as determined by syntax, i.e. either \( \lambda^\text{new}_i \leftarrow \text{SiteUpdate}(i, l_i, \lambda_i, \lambda) \), or \( (\lambda^\text{new}_i, \lambda^\text{new}) \leftarrow \text{SiteUpdate}(i, l_i, \lambda_i, \lambda) \)).

In practice, the feasibility of EP for a given posterior is essentially determined by the difficulty to evaluate, or approximate, the integral [4]. Note the simple interpretation of this quantity: this is the posterior expectation of \( t(\theta) \), for pseudo-prior \( q_{-i} \), and pseudo-likelihood the likelihood factor \( l_i(\theta) \). (In the EP literature, the pseudo-prior \( q_{-i} \) is often called the cavity distribution, and the pseudo-posterior \( \propto q_{-i}(\theta) l_i(\theta) \) the tilted or hybrid distribution.)

### 2.4 Gaussian sites

In this paper, we will focus on Gaussian approximations; that is \( Q \) is the set of Gaussian densities

\[
q_\lambda(\theta) \propto \exp \left\{ -\frac{1}{2} \theta' Q \theta + r' \theta \right\}, \quad \lambda = \left( r, -\frac{1}{2} Q \right)
\]

and EP computes iteratively a Gaussian approximation of \( \pi \), obtained as a product of Gaussian factors. For this particular family, simple calculations show that the site updates take the form given by Algorithm 2.

In words, one must compute the expectation and variance of the pseudo-posterior obtained by multiplying the Gaussian pseudo-prior \( q_{-i} \), and likelihood \( l_i \).

### 2.5 Order of site updates: sequential EP, parallel EP, and block-parallel EP

We now discuss in which order the site updates may be performed; i.e. should site updates be performed sequentially, or in parallel, or something in between.
Algorithm 2 EP Site update (Gaussian case)

Function SiteUpdate\((i, l, (r_i, Q_i), (r, Q))\):

1. Compute

\[
Z_h = \int q_{-i}(\theta)l_i(\theta)\,d\theta
\]

\[
\mu_h = \frac{1}{Z_h} \int \theta q_{-i}(\theta)l_i(\theta)\,d\theta
\]

\[
\Sigma_h = \frac{1}{Z_h} \int \theta^t q_{-i}(\theta)l_i(\theta)\,d\theta - \mu_h\mu_h^t
\]

where \(q_{-i}(\theta)\) is the Gaussian density

\[
q_{-i}(\theta) \propto \exp \left\{ -\frac{1}{2} \theta^t (Q - Q_i) \theta + (r - r_i)^t \theta \right\}.
\]

2. Return \((r_{\text{new}}^i, Q_{\text{new}}^i)\), and optionally \((r_{\text{new}}, Q_{\text{new}})\) (according to syntax as in Algorithm 1), where

\[
(Q_{\text{new}}, r_{\text{new}}) = \left( \Sigma_h^{-1}, \Sigma_h^{-1} \mu_h \right),
\]

\[
(Q_i^\text{new}, r_i^\text{new}) = (Q_i + Q_{\text{new}} - Q, r_i + r_{\text{new}} - r).
\]

The initial version of EP, as described in Minka (2001), was purely sequential (and will therefore be referred to as “sequential EP” from now on): one updates \(\lambda_0\) given the current values of \(\lambda_1, \ldots, \lambda_n\), then one updates \(\lambda_1\) given \(\lambda_0\) (as modified in the previous update) and \(\lambda_2, \ldots, \lambda_n\), and so on; see Algorithm 3. Since the function SiteUpdate \((i, l, \lambda_i, \lambda)\) computes the updated version of both \(\lambda_i\) and \(\lambda = \sum_{i=0}^n \lambda_i\), \(\lambda\) changes at each call of SiteUpdate.

Algorithm 3 Sequential EP

\begin{algorithmic}
   \REQUIRE initial values for \(\lambda_0, \ldots, \lambda_n\)
   \STATE \(\lambda \leftarrow \sum_{i=0}^n \lambda_i\)
   \REPEAT
   \FOR \(i = 0\) \TO \(n\)
   \STATE \((\lambda_i, \lambda) \leftarrow \text{SiteUpdate}\(i, l_i, \lambda_i, \lambda)\)
   \ENDFOR
   \UNTIL convergence
   \RETURN \(\lambda\)
\end{algorithmic}

Algorithm 3 is typically run until \(\lambda = \sum_{i=0}^n \lambda_i\) stabilises in some sense.

The main drawback of sequential EP is that, given its sequential nature, it is not easily amenable to parallel computation. Cseke and Heskes (2011) proposed a parallel EP algorithm, where all sites are updated in parallel, independently of each other. This is equivalent to update the sum \(\lambda = \sum_{i=0}^n \lambda_i\) only after all the sites have been updated; see Algorithm 4.
Algorithm 4 Parallel EP

Require: initial values for $\lambda_0, \ldots, \lambda_n$

$\lambda \leftarrow \sum_{i=0}^{n} \lambda_i$

repeat

for $i = 0$ to $n$ do (parallel)

$\lambda_i \leftarrow \text{SiteUpdate} (i, l_i, \lambda_i, \lambda)$

end for

$\lambda \leftarrow \sum_{i=0}^{n} \lambda_i$

until convergence

return $\lambda$

Algorithm 5 Block-parallel EP

Require: initial values for $\lambda_0, \ldots, \lambda_n$

$\lambda \leftarrow \sum_{i=0}^{n} \lambda_i$

repeat

for $k = 1$ to $\lceil (n + 1)/n_{\text{core}} \rceil$ do

for $i = (k - 1)n_{\text{core}}$ to $(kn_{\text{core}} - 1) \wedge n$ do (parallel)

$\lambda_i \leftarrow \text{SiteUpdate} (i, l_i, \lambda_i, \lambda)$

end for

$\lambda \leftarrow \sum_{i=0}^{n} \lambda_i$

end for

until convergence

return $\lambda$

Parallel EP is “embarrassingly parallel”, since its inner loop performs $(n + 1)$ independent operations. A drawback of parallel EP is that its convergence is typically slower (i.e. requires more complete passes over all the sites) than sequential EP. Indeed, during the first pass, all the sites are provided with the same initial global approximation $\lambda$, whereas in sequential EP, the first site updates allow to refine progressively $\lambda$, which makes the following updates easier.

We now propose a simple hybrid of these two EP algorithms, which we call block-parallel EP. We assume we have $n_{\text{core}}$ cores (single processing units) at our disposal. For each block of $n_{\text{core}}$ successive sites, we update these $n_{\text{core}}$ sites in parallel, and then update the global approximation $\lambda$ after these $n_{\text{core}}$ updates; see Algorithm 5.

Quite clearly, block-parallel EP generalises both sequential EP (take $n_{\text{core}} = 1$) and parallel EP (take $n_{\text{core}} = n + 1$). This generalisation is useful in any situation where the actual number of cores $n_{\text{core}}$ available in a given architecture is such that $n_{\text{core}} \ll (n + 1)$. In this way, we achieve essentially the same speed-up as Parallel EP in terms of parallelisation (since only $n_{\text{core}}$ cores are available anyway), but we also progress faster thanks to the sequential nature of the successive block updates. We shall discuss more specifically in the next section the advantage of block-parallel EP over standard parallel EP in an ABC context.

2.6 Other practical considerations

Often, the prior, which was identified with $l_0$ in our factorisation, already belongs to the approximating parametric family: $p(\theta) = q_{\lambda_0}(\theta)$. In that case, one may fix beforehand $q_0(\theta) =$
\( l_0(\theta) = p(\theta) \), and update only \( \lambda_1, \ldots, \lambda_n \) in the course of the algorithm, while keeping \( \lambda_0 \) fixed to the value given by the prior.

EP also provides at no extra cost an approximation of the normalising constant of \( \pi \): \( Z = \int_\theta \prod_{i=0}^n l_i(\theta) \, d\theta \). When \( \pi \) is a posterior, this can be used to approximate the marginal likelihood (evidence) of the model. See e.g. Barthełmy and Chopin (2014) for more details.

In certain cases, EP updates are “too fast”, in the sense that the update of difficult sites may lead to e.g. degenerate precision matrices (in the Gaussian case). One well known method to slow down EP is to perform fractional updates (Minka, 2004); that is, informally, update only a fraction \( \alpha \in (0, 1] \) of the site parameters; see Algorithm 6.

**Algorithm 6** Generic site update in EP (fractional version, requires \( \alpha \in (0, 1] \))

- **Function** SiteUpdate \((i, l_i, \lambda_i, \lambda)\):
  1. Compute
     \[
     \lambda^{\text{new}} := \alpha \lambda (E_h[t(\theta)]) + (1 - \alpha) \lambda, \quad \lambda_i^{\text{new}} := \lambda_i + \alpha \{ \lambda (E_h[t(\theta)]) - \lambda_i \}
     \]
     with \( E_h[t(\theta)] \) defined in (3), see Step 1 of [1].
  2. As Step 2 of Algorithm [1].

In practice, reducing \( \alpha \) is often the first thing to try when EP either diverges or fails because of non-invertible matrices (in the Gaussian case). Of course, the price to pay is that with a lower \( \alpha \), EP may require more iterations to converge.

### 2.7 Theoretical properties of EP

EP is known to work well in practice, sometimes surprisingly so, but it has proved quite resistant to theoretical study. In Barthełmy and Chopin (2014) we could give no guarantees whatsoever, but since then the situation has improved. The most important question concerns the quality of the approximations produced by EP. Under relatively strong conditions Dehaene and Barthełmy (2015b) were able to show that Gaussian EP is asymptotically exact in the large-data limit. This means that if the posterior tends to a Gaussian (which usually happens in identifiable models), then EP will recover the exact posterior. Dehaene and Barthełmy (2015a) show further that EP recovers the mean of the posterior with an error that vanishes in \( O(n^{-2}) \), where \( n \) is the number of data-points. The error is up to an order of magnitude lower than what one can expect from the canonical Gaussian approximation, which uses the mode of the posterior as an approximation to the mean.

However, in order to have an EP approximation, one needs to find one in the first place. The various flavours of EP (including the ones described here) are all relatively complex fixed-point iterations and their convergence is hard to study. Dehaene and Barthełmy (2015b) show that parallel EP converges in the large-data limit to a Newton iteration, and inherits the potential instabilities in Newton’s method. Just like Newton’s method, non-convergence in EP can be fixed by slowing down the iterations, as described above.

The general picture is that EP should work very well if the hybrids are well-behaved (log-concave, roughly). Like any Gaussian approximation it can be arbitrarily poor when used on multi-modal posterior distributions, unless the modes are all equivalent.
Note finally that the results above apply to variants of EP where hybrid distributions are tractable (meaning their moments can be computed exactly). In ABC applications that is not the case, and we will incur additional Monte Carlo error. As we will explain, part of the trick in using EP in ABC settings is finding ways of minimising that additional source of errors.

3 Applying EP in ABC

3.1 Principle

Recall that our objective is to approximate the ABC posterior

\[ p_{\epsilon}(\theta | y^*) \propto p(\theta) \prod_{i=1}^{n} \left\{ \int f_i(y_i | \theta) \mathbb{I}\{\|s_i(y_i) - s_i(y_i^*)\| \leq \epsilon\} \, dy_i \right\} \]

for a certain factorisation of the likelihood, and for a certain collection of local summary statistics \( s_i \). This immediately suggests using EP on the following collection of sites

\[ l_i(\theta) = \int f_i(y_i | \theta) \mathbb{I}\{\|s_i(y_i) - s_i(y_i^*)\| \leq \epsilon\} \, dy_i \]

for \( i = 1, \ldots, n \). For convenience, we focus on the Gaussian case (i.e. the \( l_i \)’s will be approximated by Gaussian factors \( q_i \)), and assume that the prior \( p(\theta) \) itself is already Gaussian, and does not need to be approximated.

From Algorithm 2, we see that, in this Gaussian case, it is possible to perform a site update provided that we are able to compute the mean and variance of a pseudo-posterior, corresponding to a Gaussian prior \( q_{-i} \), and likelihood \( l_i \).

Algorithm 7 describes a simple rejection algorithm that may be used to perform the site update. Using this particular algorithm inside sequential EP leads to the EP-ABC algorithm derived in Barthelmé and Chopin (2014). We stress however that one may generally use any ABC approach to perform such a site update. The main point is that this local ABC problem is much simpler than ABC for the complete likelihood for two reasons. First, the pseudo-prior \( q_{-i} \) is typically much more informative than the true prior \( p(\theta) \), because \( q_{-i} \) approximates the posterior of all the data minus \( y_i \). Thus, we are much less likely to sample values of \( \theta \) with low likelihood. Second, even for a fixed \( \theta \), the probability that \( \|s_i(y_i) - s_i(y_i^*)\| \leq \epsilon \) is typically much larger than \( \|s(y) - s(y^*)\| \leq \epsilon \), as \( s_i \) is generally of lower dimension than \( s \).

3.2 Practical considerations

We have observed that in many problems the acceptance rate of Algorithm 7 may vary significantly across sites, so, instead of fixing \( M \), the number of simulated pairs \( (\theta^{(m)}, y_i^{(m)}) \), to a given value, we recommend to sample until the number of accepted pairs (i.e. the number of \( (\theta^{(m)}, y_i^{(m)}) \) such that \( \|s_i(y_i^{(m)}) - s_i(y_i^*)\| \leq \epsilon \) equals a certain threshold \( M_0 \).

Another simple way to improve EP-ABC is to generate the \( \theta^{(m)} \) using quasi-Monte Carlo: for distribution \( N(\mu_{-i}, \Sigma_{-i}) \), we take \( \theta^{(m)} = \mu_{-i} + L\Phi^{-1}(u^{(m)}) \), where \( \Phi^{-1} \) is the Rosenblatt transformation (multivariate quantile function) of the unit normal distribution of dimension \( \text{dim}(\theta) \), \( LL^t = \Sigma_{-i} \) is the Cholesky decomposition of \( \Sigma_{-i} \), and the \( u^{(m)} \) is a low-discrepancy
Algorithm 7 Local ABC algorithm to perform site update

Function SiteUpdate$(i, f_i, (r_i, Q_i), (r, Q))$:

1. Simulate $\theta^{(1)}, \ldots, \theta^{(M)} \sim N(\mu_{-i}, \Sigma_{-i})$ where $\Sigma_{-i}^{-1} = Q - Q_i$, $\mu_{-i} = \Sigma_{-i}(r - r_i)$.

2. For each $m = 1, \ldots M$, simulate $y_i^{(m)} \sim f_i(\cdot | \theta^{(m)})$.

3. Compute

\[ M_{\text{acc}} = \sum_{m=1}^{M} \mathbb{I}\left\{ \|s_i(y_i^{(m)}) - s_i(y^*_i)\| \leq \epsilon \right\} \]
\[ \hat{\mu}_h = \frac{1}{M_{\text{acc}}} \sum_{m=1}^{M} \theta^{(m)} \mathbb{I}\left\{ \|s_i(y_i^{(m)}) - s_i(y^*_i)\| \leq \epsilon \right\} \]
\[ \hat{\Sigma}_h = \frac{1}{M_{\text{acc}}} \sum_{m=1}^{M} \theta^{(m)}\left[ \theta^{(m)} \right]^t \mathbb{I}\left\{ \|s_i(y_i^{(m)}) - s_i(y^*_i)\| \leq \epsilon \right\} - \hat{\mu}_h \hat{\mu}_h^t \]

4. Return $(r_i^{\text{new}}, Q_i^{\text{new}})$, and optionally $(r^{\text{new}}, Q^{\text{new}})$ (according to syntax as in Algorithm 1), where

\[ (Q_i^{\text{new}}, r_i^{\text{new}}) = \left( \Sigma_h^{-1}, \hat{\Sigma}_h^{-1} \hat{\mu}_h \right), \]
\[ (Q^{\text{new}}, r^{\text{new}}) = (Q_i + Q^{\text{new}} - Q, r_i + r^{\text{new}} - r). \]
sequence, such as the Halton sequence; see e.g. Chap. 5 in Lemieux (2009) for more background on low-discrepancy sequences and quasi-Monte Carlo.

Regarding $\epsilon$, our practical experience is that finding a reasonable value through trial and error is typically much easier with EP-ABC than with standard ABC. This is because the $y_i$'s are typically of much lower dimension than the complete data-set $y$. However, one more elaborate recipe to calibrate $\epsilon$ is to run EP-ABC with a first value of $\epsilon$, then set $\epsilon$ to the minimal value such that the proportion of simulated $y_i$ at each site such that $\|s_i(y_i) - s_i(y_i')\| \leq \epsilon$ is above, say, 5%. Then one may start over with this new value of $\epsilon$.

Another direction suggested by Mark Beaumont in a personal communication is to correct the estimated precision matrices for bias, using formula (4) from Paz and Sánchez (2015).

### 3.3 Speeding up parallel EP-ABC in the IID case

This section considers the IID case, i.e. the model assumes that the $y_i$ are IID (independent and identically distributed), given $\theta$: then

$$p(y|\theta) = \prod_{i=1}^{n} f_1(y_i|\theta)$$

where $f_1$ denotes the common density of the $y_i$. In this particular case, each of the $n$ local ABC posteriors, as described by Algorithm 7, will use pseudo-data from the same distribution (given $\theta$). This suggests recycling these simulations across sites.

Barthelmé and Chopin (2014) proposed a recycling strategy based on sequential importance sampling. Here, we present an even simpler scheme that may be implemented when Parallel EP is used. At the start of iteration $t$ of Parallel EP, we sample $\theta^{(1)}, \ldots, \theta^{(M)} \sim N(\mu, \Sigma)$, the current global approximation of the posterior. For each $\theta^{m}$, we sample $y^{(m)} \sim f_1(y|\theta^{(m)})$. Then, for each site $i$, we can compute the first two moments of the hybrid distribution by simply doing an importance sampling step, from $N(\mu, \Sigma)$ to $N(\mu_i, \Sigma_{i-})$, which is obtained by dividing the density of $N(\mu, \Sigma)$ by factor $q_i$. Specifically, the weight function is:

$$\frac{|Q_{-i}| \exp \left\{-\frac{1}{2} \theta^i Q_{-i} \theta + r_{-i}^t \theta \right\}}{|Q| \exp \left\{-\frac{1}{2} \theta^i Q \theta + r^t \theta \right\}} = \frac{|Q - Q_i|}{|Q|} \exp \left\{\frac{1}{2} \theta^i Q \theta - r_{-i}^t \theta \right\}$$

since $Q = Q_i + Q_{-i}, r = r_i + r_{-i}$. Note that further savings can be obtained by retaining the samples for several iterations, regenerating only when the global approximation has changed too much relative to the values used for sampling. In our implementation we monitor the drift by computing the Effective Sample Size of importance sampling from $N(\mu, \Sigma)$ (the distribution of the current samples) for the new global approximation $N(\mu', \Sigma')$.

We summarise the so-obtained algorithm as Algorithm 8. Clearly, recycling allows us for a massive speed-up when the number $n$ of sites is large, as we re-use the same set of simulated pairs $(\theta^{(m)}, y^{(m)})$ for all the $n$ sites. In turns, this allows us to take a larger value for $M$, the number of simulations, which leads to more stable results.

We have advocated Parallel EP in Section 2 as a way to parallelise the computations over the $n$ sites. Given the particular structure of Algorithm 8, we see that it is also easy to parallelise the simulation of the $M$ pairs $(\theta^{(m)}, y^{(m)})$ that is performed at the start of each EP iteration; this part is usually the bottleneck of the computation. In fact, we also observe that Algorithm 8
Algorithm 8 Parallel EP-ABC with recycling (IID case)

**Require:** $M$ (number of samples), initial values for $((r_i, Q_i))_{i=0, \ldots, n}$ (note $(r_0, Q_0)$ stays constant during the course of the algorithm, as we have assumed a Gaussian prior with natural parameter $(r_0, Q_0)$)

repeat
  $Q \leftarrow \sum_{i=0}^{n} Q_i$, $r \leftarrow \sum_{i=0}^{n} r_i$, $\Sigma \leftarrow Q^{-1}$, $\mu \leftarrow \Sigma r$
  for $m = 1, \ldots, M$ do
    $\theta^{(m)} \sim N(\mu, \Sigma)$
    $y^{(m)} \sim f_1(y|\theta^{(m)})$
  end for
  for $i = 1, \ldots, n$ do
    for $m = 1, \ldots, M$ do
      $w^{(m)} \leftarrow |Q - Q_i| \exp \left\{ \frac{1}{2} (\theta^{(m)})^t Q \theta^{(m)} - r_i^t \theta^{(m)} \right\} \mathbb{1}\{\|s_i(y^{(m)}_i) - s_i(y^*_i)\| \leq \epsilon\}$
    end for
    $\hat{Z} \leftarrow M^{-1} \sum_{m=1}^{M} w^{(m)}$
    $\hat{\mu} \leftarrow (M \hat{Z})^{-1} \times \sum_{m=1}^{M} w^{(m)} \theta^{(m)}$
    $\hat{\Sigma} \leftarrow (M \hat{Z})^{-1} \times \sum_{m=1}^{M} w^{(m)} \theta^{(m)} \left[ \theta^{(m)} \right]^t - \hat{\mu} \hat{\mu}^t$
    $r_i \leftarrow \hat{\Sigma}^{-1} \hat{\mu} - r_i$
    $Q_i \leftarrow \hat{\Sigma}^{-1} - Q_i$
  end for
until Stopping rule (e.g. changes in $(r, Q)$ have become small)

performs slightly better than the recycling version of EP-ABC (as described in Barthelmé and Chopin 2014) even on a non-parallel architecture.

4 Application to spatial extremes

We now turn our attention to likelihood-free inference for spatial extremes, following Erhardt and Smith (2012), see also Prangle (2014).

4.1 Background

The data $y$ consist of $n$ IID observations $y_i$, typically observed over time, where $y_i \in \mathbb{R}^d$ represents some maximal measure (e.g. rainfall) collected at $d$ locations $x_j$ (e.g. in $\mathbb{R}^2$). The standard modelling approach for extremes is to assign to $y_i$ a max-stable distribution (i.e. a distribution stable by maximisation, in the same way that Gaussians are stable by addition). In the spatial case, the vector $y_i$ is composed of $d$ observations of a max-stable process $x \rightarrow Y(x)$ at the $d$ locations $x_j$. A general approach to defining max-stable processes is (Schlather 2002):

$$Y(x) = \max_k \{s_k \max (0, Z_k(x))\}$$

where $(s_k)_{k=1}^{\infty}$ is the realisation of a Poisson process over $\mathbb{R}^+$ with intensity $\Lambda(ds) = \mu^{-1} s^{-2} ds$ (if we view the Poisson process as producing a random set of “spikes” on the positive real line, then $s_1$ is the location of the first spike, $s_2$ the second, etc.), $(Z_k)_{k=1}^{\infty}$ is a countable collection
of IID realisations of a zero-mean, unit-variance stationary Gaussian process, with correlation function $\rho(h) = \text{Corr}(Z_k(x), Z_k(x'))$ for $x, x'$ such that $\|x - x'\| = h$, and $\mu = \mathbb{E}\left[\max (0, Z_k(x))\right]$. Note that $Y(x)$ is marginally distributed according to a unit Fréchet distribution, with CDF $F(y) = \exp(-1/y)$.

As in Erhardt and Smith (2012), we will consider the following parametric Whittle-Matérn correlation function

$$
\rho_\theta(h) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{h}{c}\right)^\nu K_\nu\left(\frac{h}{c}\right), \quad c, \nu > 0
$$

where $K_\nu$ is the modified Bessel function of the third kind. We take $\theta = (\log \nu, \log c)$ so that $\Theta = \mathbb{R}^2$. (We will return to this logarithmic parametrisation later.)

The main issue with spatial extremes is that, unless $d \leq 2$, the likelihood $p(y|\theta)$ is intractable. One approach to estimate $\theta$ is pairwise marginal composite likelihood (Padoan et al., 2010). Alternatively, (5) suggests a simple way to simulate from $p(y|\theta)$, at least approximately (e.g. by truncating the domain of the Poisson process to $[0, S_{\text{max}}]$). This motivates likelihood-free inference (Erhardt and Smith, 2012).

4.2 Summary statistics

One issue however with likelihood-free inference for this class of models is the choice of summary statistics: Erhardt and Smith (2012) compare several choices, and find that the one that performs best is some summary of the clustering of the $d(d-1)(d-2)/6$ triplet-wise coefficients

$$
\sum_{i=1}^n \{\max(y_i(x_j), y_i(x_k), y_i(x_l))\}, \quad 1 \leq j < k < l \leq d.
$$

But computing these coefficients require $O(d^3)$ operations, and may actually be more expensive than simulating the data itself. Prangle (2014) observes in a particular experiment than the cost of computing these coefficients is already more that twice the cost of simulating data for $d = 20$. As a result, the overall approach of Erhardt and Smith (2012) may take several days to run on a single-core computer.

In contrast, EP-ABC allows us to define local summary statistics, $s_i(y_i)$, that depend only on one data-point $y_i$. We simply take $s_i(y_i)$ to be the (2-dimensional) OLS (ordinary least squares) estimate of regression

$$
\log |F(y_i(x_j)) - F(y_i(x_k))| = a + b \log \|x_j - x_k\| + \epsilon_{jk}, \quad 1 \leq j < k \leq d
$$

where $F$ is the unit Fréchet CDF. The madogram function $h \rightarrow \mathbb{E}[|Y(x) - Y(x')|]$, for $\|x - x'\| = h$, or its empirical version, is a common summary of spatial dependencies (for extremes). Here, we take the $F-$madogram, i.e. $Y(x)$ is replaced by $F(Y(x)) \sim U[0, 1]$, because $Y(x)$ is Fréchet and thus $\mathbb{E}[|Y(x)|] = +\infty$.

4.3 Numerical results on real data

We now apply EP-ABC to the rainfall dataset of the SpatialExtremes R package (available at http://spatialextremes.r-forge.r-project.org/), which records maximum daily rainfall amounts over the years 1962–2008 occurring during June–August at 79 sites in Switzerland. We ran sequential EP with recycling and quasi-Monte Carlo (see discussion in Section 3.2). Figure
Figure 1: 50% credible ellipses of the Gaussian approximation of the posterior computed by EP-ABC, for different values of $\epsilon$, and rainfall dataset.

1 plots the EP-ABC posterior for $\epsilon = 0.2, 0.05$ and $0.02$. A $N(0,1)$ prior was used for both components of $\theta = (\log \nu, \log c)$.

Each run took about 3 hours on our desktop computer, and generated about $10^5$ data-points (i.e. realisations $y_i \in \mathbb{R}^d$, where $d$ is the number of stations). As a point of comparison, we ran Erhardt and Smith (2012)'s R package for a week on the same computer, which led to the generation of $5 \times 10^4$ complete datasets (i.e. $\approx 4 \times 10^6$ data-points). However, the ABC posterior approximation obtained from the 100 generated datasets that were closest to the data, relative to their summary statistics, was not significantly different from the prior.

Finally, we discuss the strong posterior correlations between the two parameters that are apparent in Figure 1. Figure 2 plots a heat map of functions $(\nu, c) \rightarrow \int |\rho_{\nu,c} - \rho_{\nu_0,c_0}|$ and $(\log \nu, \log c) \rightarrow \int |\rho_{\nu,c} - \rho_{\nu_0,c_0}|$, for $(\nu_0, c_0) = (8, 4)$. The model appears to be nearly non-identifiable, as values of $(\nu, c)$ that are far away may produce correlation functions that are nearly indistinguishable. In addition, the parametrisation $\theta = (\log \nu, \log c)$ has the advantage of giving an approximately Gaussian shape to contours, which is clearly helpful in our case given that EP-ABC generates a Gaussian approximation. Still, it is interesting to note that EP-ABC performs well on such a nearly non-identifiable problem.

4.4 EP Convergence

Finally, we compare the convergence (relative to the number of iterations) of the standard version, and the block-parallel version (described in Section 2.5) of EP-ABC, on the rainfall dataset discussed above. Figure 3 plots the evolution of the posterior mean of both parameters $\nu$ (left panel) and $c$ (right panel), relative to the number of site updates, for 3 runs of both versions, and for $\epsilon = 0.05$.

We took $n_{\text{core}} = 10$ (i.e. blocks of 10 sites are updated in parallel), although both algorithms were run on a single core. We see that both algorithms essentially converge at the same rate.
Figure 2: Heat map of functions $(\nu, c) \rightarrow \int |\rho_{\nu,c} - \rho_{\nu_0, c_0}|$ and $(\log \nu, \log c) \rightarrow \int |\rho_{\nu,c} - \rho_{\nu_0, c_0}|$, for $(\nu_0, c_0) = (8, 4)$.

Figure 3: Posterior mean of $\log \nu$ (left panel) and $\log c$ (right panel) as a function of the number of passes (one pass equals $n = 47$ site updates), for 3 runs of the sequential version (solid grey line), and block-parallel version ($n_{\text{core}} = 10$, dashed black line) of EP-ABC, applied to rainfall dataset ($\epsilon = 0.05$).

Thus, if implemented on a 10-core machine, the block-parallel version should offer essentially a $\times 10$ speed-up.

5 Conclusion

Compared to standard ABC, the main drawback of EP-ABC is that it introduces an extra level of approximation, because of its EP component. On the other hand, EP-ABC strongly reduces, or sometimes removes entirely, the bias introduced by summary statistics, as it makes possible to use $n$ local summaries, instead of just one for the complete dataset. In our experience (see e.g. the examples in Barthelmé and Chopin (2014)), this bias reduction more than compensates the bias introduced by EP. But the main advantage of EP-ABC is that it is much faster than standard ABC. Speed-ups of more than 100 are common, as evidenced by our spatial extremes example.

We have developed a Matlab package, available at https://sites.google.com/site/
that implements EP-ABC for several models, including spatial extremes. The current version of the package includes the parallel version described in this paper.

An interesting direction for future work is to integrate current developments on model emulators into EP-ABC. Model emulators are ML algorithms that seek to learn a tractable approximation of the likelihood surface from samples (Wilkinson [2014]). A variant directly learns an approximation of the posterior distribution, as in Gutmann and Corander [2015]. Heess et al. [2013] introduce a more direct way of using emulation in an EP context. Their approach is to consider each site as a mapping between the parameters of the pseudo-prior and the mean and covariance of the hybrid, and to learn the parameters of that mapping. In complex but low-dimensional models typical of ABC applications this viewpoint could be very useful and deserves to be further explored.

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