Web-based Supplementary Materials for “Efficient estimation and prediction for the Bayesian binary spatial model with flexible link functions”

by

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Web Appendix A

Further details on the simulations

The data are simulated from the following model, where the sampled locations \( s_i = (s_{i,1}, s_{i,2}) \), \( i = 1, \ldots, 100 \) are shown in Web Figure 1.

\[
Y(s_i)|z(s_i) \sim \text{Binomial}(250, p(s_i)), \\
h_\nu(p(s_i)) = z(s_i), \\
Z(s_i) \sim \text{GRF}(\mu(s_i), \tau^2 + \sigma^2 \rho(u; \phi)), \\
\mu(s_i) = \beta_0 + \beta_1 \times 1(s_{i,1} > 0.5).
\]

In the above \( \text{GRF}(\mu(s), c(u)) \) denotes the distribution of the Gaussian random field with mean at the spatial location \( s \mu(s) \) and covariance function \( c(u) \). We set \( \beta_0 = 1.70, \beta_1 = -3.40, \tau^2 = 0.20, \sigma^2 = 1.00, \rho(u; \phi) \) to be the Matérn correlation function with \( \kappa = 0.5 \) and \( \phi \) and \( \nu \) varying according to Web Table 1.

The following models were considered for fitting the data

- **EB** Robit link fitted by EB with skeleton points as in Web Table 1;
- **MCLg U** Logit link with Uniform(0, 1.5) prior for \( \phi \);
- **MCLg Ex** Logit link with Exponential(\( \phi \)) prior for \( \phi \);
- **MCLg HN** Logit link with Half-Normal(mean = \( \phi \)) prior for \( \phi \);
- **MCLg IG** Logit link with Inverse-Gamma(shape = 1, scale = 1) prior for \( \phi \);
- **MCPr U** Probit link with Uniform(0, 1.5) prior for \( \phi \);
- **MCPr Ex** Probit link with Exponential(\( \phi \)) prior for \( \phi \);
- **MCPr HN** Probit link with Half-Normal(mean = \( \phi \)) prior for \( \phi \);
- **MCPr IG** Probit link with Inverse-Gamma(shape = 1, scale = 1) prior for \( \phi \).
Web Figure 1 – Sampling locations for the simulations.

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<th>0.2 or 0.6</th>
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<td>$\nu$ true</td>
<td>0.5, 1.0, 4.0</td>
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<tr>
<td>$\nu$ skeleton</td>
<td>$\nu \cdot (0.5, 0.6, 0.8, 1.0, 1.2, 1.6, 2.0) (4, 6, 8, 12, 15)$</td>
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Web Table 1 – Skeleton points for the EB method for the simulations. In the table, the $\phi$ and $\nu$ factors correspond to their true values.

In addition, the following priors were assumed for all models

$$\beta_j | \sigma^2 \sim^{\text{ind}} N(0, 100\sigma^2), \text{ for } j = 0, 1,$$
$$\sigma^2 \sim \chi^2_{ScI}(1, 1).$$

Prediction is considered at a $11 \times 11$ square grid covering the sampling domain and a prediction score is computed for each method. The total computing time for each combination of parameters including all 100 repetitions was between 7 to 9 hours on a computer with Intel(R) Core(TM) i5-2500 CPU, 3.30GHz processor and 4Gb RAM. Web Tables 2–6 show the results derived from 100 simulations corresponding to a new simulated $z$ and $y$ each time.
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Web Table 2 – Estimates (first row) and RMSE (second row) of the spatial range parameter $\phi$ under each model.

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Web Table 3 – Estimates (first row) and RMSE (second row) of the spatial sill parameter $\sigma^2$ under each model. The true parameter value is $\sigma^2 = 1$. 

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Web Table 4 – Estimates (first row) and RMSE (second row) of the parameter $\beta_0$ under each model. The true parameter value is $\beta_0 = 1.70$.

$\phi = 0.6$

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</tr>
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<td>1.77</td>
<td>0.94</td>
<td>0.70</td>
<td>0.43</td>
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</table>

Web Table 5 – Estimates (first row) and RMSE (second row) of the parameter $\beta_1$ under each model. The true parameter value is $\beta_1 = -3.40$. 

4
Web Table 6 – Prediction score (first row) and standard deviation of the score (second row) under each model.
Web Appendix B

Detailed analysis of the Celastrus Orbiculatus data

The data consist of the presence/absence of the *C. Orbiculatus* species at 603 locations. Web Figure 2 shows the sampling locations along with the presence/absence of the species. The following environmental variables were also used as predictors:

**HabitatClass** The current state of the habitat: a factor variable of four levels;

**LULCChange** Land use and land cover (LULC) change: a factor of 5 levels;

**cat1970** What the land use category was in 1970: a factor of 6 levels;

**CanopyClosure** An ordinal score for the proportion of sky blocked by a canopy of leaves;

**HeavilyManagedPts** A binary indicator where 1 means heavy land management, e.g. a paved area or a lawn;

**LogEdgeDistance** The distance (in feet) of the plot to a vegetation edge, such as a forest in the logarithmic scale.

The first three variables are treated as factors and the last three as numerical. An intercept was also included, totaling $m = 16$ regression coefficients.

![Web Figure 2 – Sampled locations for the *C. Orbiculatus* example.](image)

Let $y_i$ denote the presence/absence of the *C. Orbiculatus* species at location $s_i$ and $Z(s)$ be the spatial process denoting the intensity of occurrence. We also denote by $f_j(s)$ the value of the $j$th
regression variable at location $s$. The following hierarchical model is used.

$$
Y_i | z_i \sim \text{Bin}(1, p_i),
$$

$$
h_\nu(p_i) = z_i,
$$

$$
Z(s) \sim \text{GRF} \left( \sum_{j=1}^{m} \beta_j f_j(s), \sigma^2 \rho(u; \phi) \right),
$$

$$
\beta_j | \sigma^2 \text{ ind} \sim N(0, 1000 \sigma^2), \ j = 1, \ldots, m,
$$

$$
\sigma^2 \sim \chi^2_{\text{ScI}}(4, 0.5).
$$

In the above $\text{GRF}(\mu(s), c(u))$ denotes the distribution of the Gaussian random field with mean at the spatial location $s \mu(s)$ and covariance function $c(u)$. We fix $\rho(u; \phi)$ to the exponential correlation function, i.e. Matérn with $\kappa = 0.5$.

We consider the case where $h_\nu$ is the robit($\nu$), logit and probit link function. The model is fitted by both an empirical Bayes (EB) and a full Bayesian (FB) method. The unknown parameters consist of $\beta_j$, $\sigma^2$, $\phi$ and, in the case of the robit link, $\nu$. For the EB method, the skeleton set for $(\phi, \nu)$ was set to

$$(\phi, \nu) \in \{1, 3, 5\} \times \{2, 4, 6\},$$

for the robit model, while for the logit and probit models only the part which corresponds to $\phi$ was used.

From the whole data set, 200 observations were randomly selected and the absence/presence was assumed unobserved. Each model was fitted using the remaining 403 observations and prediction is considered at the deleted 200 locations. A prediction score is then calculated as discussed in the main paper. Web Table 7 shows the parameter estimates obtained by each model as well as the prediction score. For comparison, we show the estimates obtained when all 603 observations are used in the case of the robit model.

Web Figure 3 shows the distribution of the posterior samples using each method for the parameters $\beta$ and $\sigma^2$. The results from using EB or FB to fit the same model overlap substantially.

Using the fitted robit model with complete data, we consider prediction at a fine square grid covering the sampling domain. The predicted probability of presence is depicted in Web Figure 4. The figure shows that it is more likely to find the species at the southern part of the domain. It is evident that at some parts where the predicted probability is extreme, some observations appear as outliers.
## Web Table 7 – Parameter estimates for the *C. Orbiculatus* example from different models.

EB denotes a model fitted by empirical Bayes and FB a model fitted by full Bayes. Rb, Lg, Pr are the robit, logit and probit link functions respectively and Compl means the complete data set was used.

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<th>Rb EB</th>
<th>Lg EB</th>
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Web Figure 3 – Posterior samples for $\beta$ and $\sigma^2$ under different methods. Methods A–F correspond to the columns of Table 7.
Web Figure 4 – Predicted probability of occurrence for the *C. Orbiculatus* species.
Web Appendix C

Illustration of the choice for the skeleton points for the Rhizoctonia example

The Rhizoctonia root rot is a disease that affects the roots of plants by hindering their process of absorbing water and nutrients from soil. This example was first considered in Zhang (2002): 15 plants were selected from each of \( n = 100 \) randomly chosen locations in a farm and the number of crown roots and infected crown roots were counted. For the purpose of treating the disease and site-specific farming, we wish to predict the random field over the whole area. As in Zhang (2002), we assume that the number of infected crown roots \( Y(s_i) \) at site \( s_i \) has a Binomial \( (\ell_i, p_i) \) distribution, where \( \ell_i \) is the total number of crown roots at site \( s_i \) and \( p_i \) is the varying binomial success parameter. Following Zhang (2002) we also assume a constant mean and a spherical correlation function with unknown nugget effect for the underlying Gaussian random field.

A binomial spatial model with robit link is fitted. We use the same prior on \((\beta, \sigma^2)\) as is discussed in the main text. For the estimation of \( \xi \equiv (\phi, \nu, \omega) \) by our proposed EB method, where \( \omega = \tau^2/\sigma^2 \), we start with the following 27 skeleton points,

\[
(\phi, \nu, \omega) \in \{100, 140, 180\} \times \{3, 8, 15\} \times \{0, 0.5, 1\}.
\] (2)

The parameter \( \omega \) is known as the relative nugget parameter. We use the reverse logistic regression method using an MCMC sample of size 800, which is taken collecting every 10th sample after discarding initial 1,000 samples. A fresh MCMC sample of size 200 is subsequently drawn for the purpose of computing \( B_{\xi, \xi_1} \) for all other values of \((\phi, \nu, \omega)\) with \( \xi_1 \equiv (\phi_1, \nu_1, \omega_1) = (100, 3, 0) \). We use the asymptotic standard errors using batch means derived in Roy et al. (2015) to calculate the standard errors of our Bayes factor estimator \( \hat{B}_{\xi, \xi_1}(\hat{r}) \). In Web Figure 5 we plot the profile of the standard errors, that is, the maximum of the standard errors over the free parameter is plotted against the fixed values of the other two parameters. From Web Figure 5 we see that the variance is large when \( \nu \) is around 5, also when \( \omega \) is large. The largest standard error is around \( 2.7 \times 10^8 \).

Roy et al. (2015) also provides batch means estimates of the variance covariance matrix of \( \hat{r} \) based on the first stage samples only. We notice that the maximum variance estimates of the \( \hat{r}_i \)’s is around \( 3.7 \times 10^6 \) and the maximum is attained at the skeleton point \((140, 3, 1)\). Next, we change
the reference point from $\xi_1 \equiv (\phi_1, \nu_1, \omega_1) = (100, 3, 0)$ to $\xi_1 = (140, 3, 1)$. In this case, the maximum variance estimates of the $\hat{r}_i$’s drastically reduces to 0.45 and the plot the standard errors of $\hat{B}_{\xi, \xi_1}(\hat{r})$ is given in Web Figure 6. Finally, we change the skeleton points to

$$(\phi, \nu, \omega) \in \{100, 140, 180\} \times \{3, 5, 8, 15\} \times \{0.5, 1, 2\}, \quad (3)$$

that is, we include $\nu = 5$ in the skeleton set and replace $\omega = 0$ with $\omega = 2$. Web Figure 7 shows the plot of the standard errors of $\hat{B}_{\xi, \xi_1}(\hat{r})$. We used the same sample size as before, that is, 800 MCMC samples in the first stage and 200 samples in the second stage, but with the set of skeleton points given in (3), the maximum standard error has reduced from about $2.7 \times 10^8$ to 2.27. In Web Figure 8 we show the profile of the Bayes factors with respect to each of the parameters, that is, one of the parameters is kept fixed and the maximum of the Bayes factors over the other two parameters is plotted against the values of the first parameter. The maximum is obtained at $\hat{\phi} = 146.22$, $\hat{\nu} = 30.00$, and $\hat{\omega} = 0.95$. Web Figure 8 suggests that probit link can be used for analyzing this data set. Although, the skeleton points given in (2) resulted in large standard errors for the Bayes factor estimates, the EB estimate of the parameters $\xi$ was similar with $(\hat{\phi}, \hat{\nu}, \hat{\omega}) = (146.32, 30.00, 0.97)$. The corresponding profile plot of the Bayes factors estimates is given in Web Figure 9.

Treating these estimates $(\hat{\phi}, \hat{\nu}, \hat{\omega})$ as fixed, we subsequently estimate the other parameters of the model by running a new MCMC chain of length 1,000 collecting every 10th sample after an initial burnin of 1,000 sample. The estimates obtained are $\hat{\beta} = -1.05$ and $\hat{\sigma}^2 = 0.13$ and the 95% prediction intervals of $\beta$ and $\sigma^2$ are given by $(-1.207, -0.895)$ and $(0.092, 0.172)$ respectively. The prediction of the random field and a plot of estimated prediction uncertainty are shown in Web Figure 10. The standard errors estimates for the posterior means of $\beta$ and $\sigma^2$ are obtained using the method of overlapping batch means and equal 0.0003 and 0.0001 respectively.

In comparison with the results of Zhang (2002), who used the logit link function, our prediction has the same pattern and the same range of prediction values. (Note that Web Figure 7 in Zhang (2002) is without the mean.) We also get a similar estimate for the range but our estimate for the partial sill is 0.13 compared to Zhang’s 0.18 and the nugget to sill ratio is estimated by our method to be about 1 compared to around 2 in Zhang (2002).
Web Figure 7 – Standard errors (in log scale) of the Bayes factor estimates.

Web Figure 8 – Profile of $B_{(\nu,\phi,\omega), (\nu_1,\phi_1,\omega_1)}$ for the Rhizoctonia data with respect to each parameter corresponding to the skeleton set (3). The plot suggests a probit link, $\phi$ around 146 and $\tau^2/\sigma^2$ around 0.95.

**Web Appendix D**

**R code for analysis of the Rhizoctonia data**

Below we provide the R code for an illustrative analysis of the Rhizoctonia data. More examples can be found in demo(package = “geoBayes”).

```r
## Load the relevant R package
library(geoBayes)

## Sample size for the MCMC algorithm
Nout <- 1000
Nthin <- 10
Nbi <- 1000
```

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Web Figure 9 – Profile of $B_{(\nu, \phi, \omega), (\nu_1, \phi_1, \omega_1)}$ for the Rhizoctonia data with respect to each parameter corresponding to the skeleton set (2).

Web Figure 10 – Estimated means (left plot) and uncertainty defined as the length of 95% prediction interval divided by 4 (right panel) for the predictive distribution of the Gaussian random field for the Rhizoctonia data. The dots in the plots indicate observed locations.

```r
## Parameters for the model
kappa <- 0
ssqdf <- 1
ssqsc <- 1
betm0 <- 0
betQ0 <- .01

## Skeleton set
philist <- c(100, 140, 180)
dftlist <- c(3, 5, 8, 15)
nsqlist <- c(.5, 1, 2)
parlist <- expand.grid(phi=philist, dft=dftlist, nsq=nsqlist)
```
## Draw MCMC samples corresponding to each parameter combination in the skeleton set
runsa <- list()
for (i in 1:nrow(parlist)) {
    runsa[[i]] <- mcsglmm(Infected ~ 1, "binomial", data = rhizoctonia,
        Total, ~ Xcoord + Ycoord,
        Nout = Nout, Nthin = Nthin, Nbi = Nbi, betm0 = betm0, 
        betQ0 = betQ0, ssqdf = ssqdf, ssqsc = ssqsc, 
        corrfcn = "sph", kappa = kappa, linkp = parlist$dft[i], 
        phisc = 0, omgsc = 0, phistart = parlist$phi[i], 
        omgstart = parlist$nsq[i])
}

## Estimate the Bayes factors at the skeleton points by reverse logistic method
## and compute the importance weights for each sample (required in the second stage).
bfrl <- bfiskel(runsa, reference = 14)

## Compute contour and plot profile Bayes factors
phivec <- seq(90, 200, len=21)
dftvec <- seq(3, 30, len=21)
nsqvec <- seq(0.5, 2, .25)
bfcontour <- bf2new(bfrl, dftvec, phivec, nsqvec)
plotbf2(bfcontour, c("linkp", "phi", "omg"))

## Estimate nu, phi, omega
paroptim <- list(linkp = c(3, 15, 30), phi = c(90, 150, 200), omg = c(0, .9, 2))
pareb <- bf2optim(bfrl, paroptim)

## Sample the remaining parameters conditioned on the EB estimates
samEB <- mcsglmm(Infected ~ 1, "binomial", data = rhizoctonia,
        Total, ~ Xcoord + Ycoord,
        Nout = Nout, Nthin = Nthin, Nbi = Nbi, betm0 = betm0, 
        betQ0 = betQ0, ssqdf = ssqdf, ssqsc = ssqsc, 
        corrfcn = "sph", kappa = kappa, linkp = pareb$par["linkp"], 
        phisc = 0, omgsc = 0, phistart = pareb$par["phi"], 
        omgstart = pareb$par["omg"])

References
