

Bayesian Melding of a Forest Ecosystem Model with Correlated Inputs

Philip J. Radtke, Thomas E. Burk, and Paul V. Bolstad

ABSTRACT. Bayesian melding, a method for assessing uncertainties in deterministic simulation models, was augmented to make use of prior knowledge about correlations between model inputs. The augmentation involved the use of a nonparametric correlation induction algorithm. The modified Bayesian melding technique was applied to the process-based forest ecosystem computer model PnET-II. The Bayesian posterior distribution for this analysis did not reflect prior knowledge of input correlations for five input pairs tested unless the correlations were explicitly accounted for in the Bayesian prior distribution. For other input pairs not known to be correlated prior to the analysis, numerous significant posterior correlations were identified. For one such pair of model inputs, a moderate posterior correlation was substantiated by empirical evidence that had not previously been taken into consideration. We conclude that, when possible, efforts should be made to account for prior knowledge of correlated inputs; however, Bayesian melding may elucidate input correlations in its posterior sample, even when no prior knowledge of such correlations exists. *For. Sci.* 48(4):701–711.

Key Words: Bayesian melding, big leaf model, simulation, model evaluation, process model, Latin hypercube.

THE USE OF PROCESS-BASED forest ecosystem computer models has become commonplace for conducting research in the study of forest ecosystem dynamics. Researchers have adopted the process-based modeling paradigm because it has some key advantages over traditional statistical modeling techniques. Chief among these are the strengths of process-based models in the areas of knowledge synthesis and predictive extrapolation. Still, widespread adoption of process-based models for practical applications has been limited, mainly due to the lack of answers regarding the magnitudes of prediction uncertainty. Increasingly, attention has been paid to the need for quantitative assessments of the quality of predictions made with process-based computer models (Cipra 2000, Mäkelä et al. 2000).

Bayesian melding (BYSM) is a technique that allows for the assessment of uncertainty in deterministic computer model predictions by estimating Bayesian posterior distributions of model inputs and outputs. As such, significant potential exists to use BYSM for quantifying prediction

uncertainty in process-based forest ecosystem models. The method was developed by Raftery et al. (1995) to account for available information and uncertainty related to computer model predictions of a population of an endangered whale species. The goal of their analysis was to develop probabilistic statements of how likely it would be that the whale population might drop below some critical level following a proposed harvest of whales by aboriginal subsistence hunters. To achieve this goal, the researchers developed the theoretical framework and an algorithm for implementing what they called Bayesian synthesis.

Wolpert (1995) pointed out that Bayesian synthesis was subject to Borel's paradox, meaning results were not invariant to rescaling of model outputs. Bayesian melding was developed to overcome this limitation (Poole and Raftery 2000). The key result of BYSM is an approximation to the Bayesian joint posterior distribution for model inputs. The propagation of this distribution through the model results in the posterior distribution of outputs. Descriptive statistics—

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modes, means, variances, intervals, etc.—can be readily estimated from the posterior distributions of any subset of model inputs or outputs. Because statistics based on regions of highest Bayesian posterior density are generalized maximum likelihood estimates (Berger 1985 p. 140–143), the development of BYSM represents something of a breakthrough in research on assessing the quality of process-model predictions.

To date, researchers have conducted BYSM analyses making a simplifying assumption in their formulations of Bayesian prior distributions: that model inputs are independent of one another. BYSM does not require this assumption, but it has typically been adopted to simplify implementation of the method where input relationships were unknown or where joint prior distributions for model inputs were difficult to formulate explicitly (Raftery et al. 1995, Green et al. 1999, Poole and Raftery 2000). Interestingly, the results of BYSM analysis have been shown to elucidate relationships that exist between model inputs *a posteriori* (Green et al. 1999). Still, in many situations, prior information about relationships between model inputs is known. It would seem desirable to make use of such information when available. Ignoring relationships between model parameters can be a serious source of error in analyses that evaluate the quality of model predictions (Iman and Conover 1982, Guan 2000).

The objective here was to augment BYSM methodology to take *a priori* account of correlations known to exist between the inputs of a process-based computer model. This augmentation would be developed and applied by conducting BYSM for the process-based forest ecosystem model PnET-II (Aber et al. 1995). PnET-II was designed to address questions involving regional, long-term dynamics of ecosystem water and carbon cycling. Because of this, PnET-II has played a significant role in the modeling of regional forest ecosystem dynamics and responses to predicted climate change scenarios (McNulty et al. 1996, Goodale et al. 1998, Ollinger et al. 1998). A good deal is known about the distributions of PnET-II model inputs, including empirical evidence of correlations between some input pairs (Radtke et al. 2001).

The central question here is whether or not BYSM will accurately predict correlations between PnET-II model inputs in the posterior distribution, even though the prior distributions of inputs are assumed to be independent. We proposed to answer this question by conducting BYSM assuming independence of inputs, and comparing results to BYSM conducted assuming a prior correlation structure. The hypothesis to be tested from this approach was that BYSM posteriors would reflect correlations correctly, even when such correlations were not specified *a priori*.

Methods

BYSM was so named because of the prominence of Bayes' theorem in the methodology and the fact that the technique combines or “melds” information from three sources in deriving its estimates of Bayesian posterior distributions (Poole and Raftery 2000). Sources of information are categorized as either *direct* or *indirect*, with the third source of

information being the model itself. Direct and indirect sources are distinguished by whether they are observed directly on a population of interest or obtained from outside sources somehow related to the population of interest. Direct and indirect information may pertain to either model inputs or outputs. Direct information typically involves a sample of observations made on the population of interest. Indirect information is expressed as probability density functions (PDFs) that reflect knowledge and uncertainty about the various model quantities.

BYSM

BYSM is concerned with deterministic simulation models, particularly model inputs and outputs and functions thereof. A brief description is included here for clarity and completeness. For additional detail and examples see Raftery et al. (1995), Green et al. (1999), and Poole and Raftery (2000). A basic premise of BYSM is that information is available for some inputs and outputs, but there is likely to be some uncertainty associated with that information. The sets of model inputs and outputs *for which we have information independent of the model* are denoted by θ and ϕ , respectively, which are vectors for models that involve multiple inputs and outputs. Quantities of interest are not limited to θ and ϕ . Indirect information translates to Bayesian priors, and direct information translates to likelihoods. The premodel Bayesian prior density for inputs is denoted $q_\theta(\theta)$ and the Bayesian prior density for outputs is denoted $q_\phi(\phi)$. Both $q_\theta(\theta)$ and $q_\phi(\phi)$ are established before any execution of the model is carried out. Likelihoods for inputs and outputs are denoted $L_\theta(\theta)$ and $L_\phi(\phi)$, respectively. Subscripts θ and ϕ refer to model inputs and outputs, respectively. If we assume that information about outputs is independent of information about the inputs, Bayes' theorem gives us the following posterior distribution.

$$p(\theta, \phi) \propto q_\theta(\theta) L_\theta(\theta) q_\phi(\phi) L_\phi(\phi) \quad (1)$$

Although (1) is a posterior in the Bayesian sense, it is compiled without any consideration of the information contained in the model; thus, $p(\theta, \phi)$ is referred to as the joint *pre-model* (posterior) distribution of θ and ϕ .

The model can be thought of as a mapping of inputs to outputs: $\Phi(\theta) \rightarrow \phi$. It follows that the joint *post-model* (posterior) distribution $\pi(\theta, \phi)$ will have nonzero probability only when $\phi = \Phi(\theta)$. Raftery et al. (1995) defined the joint distribution of θ and ϕ given the model as “the restriction of the pre-model distribution to the submanifold $\{(\theta, \phi): \phi = \Phi(\theta)\}$,” namely

$$\pi(\theta, \phi) \propto \begin{cases} p(\theta, \Phi(\theta)) & \text{if } \phi = \Phi(\theta) \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

Resolving Borel's Paradox

In implementing Bayesian synthesis, Raftery et al. (1995) used the sampling importance resampling (SIR) algorithm of Rubin (1988) to approximate $\pi(\theta, \phi)$ so that inferences on the post-model marginal distributions of inputs and outputs could be made. Wolpert (1995) pointed out that the joint distribu-

tion $\pi(\theta, \phi)$ in Equation (2) did not exist because of Borel's paradox. This paradox arises in BYSM because $q_\theta(\theta)$, when propagated through the model, implies a prior distribution on the model outputs denoted $q_\theta^i(\phi)$ and referred to as the prior distribution of outputs implied by the model and $q_\theta(\theta)$. Nothing in the method constrains $q_\theta^i(\phi)$ and $q_\phi(\phi)$ to be equal, effectively allowing for two conflicting priors to exist simultaneously. Raftery et al. (1996) proposed a modification to the method to eliminate Borel's paradox. Their solution involved logarithmic pooling of the specified and implied priors into a single pooled prior for model outputs

$$\tilde{q}^{[\phi]}(\phi) \propto q_\theta^i(\phi)^\alpha q_\phi(\phi)^{1-\alpha} \quad (3)$$

where α is a pooling weight $0 \leq \alpha \leq 1$. When the two priors on the right hand side of (3) arise from the same base of expertise, a logical choice for α is 0.5. Other choices may be appropriate if input and output priors are based on different expertise bases and one expert is seen as more reliable than the other (Poole and Raftery 2000). When $\alpha = 0.5$ is chosen, Equation (3) amounts to geometric pooling of the specified and implied priors for model outputs.

Assuming that inferences are to be made on inputs, the same problem arises because $q_\phi(\phi)$, when propagated through the inverted model, implies a prior distribution on inputs that will surely contradict $q_\theta(\theta)$. The problem is further complicated when the model is not invertible, a certainty for models in which the number of outputs is smaller than the number of inputs. The ideal solution involves obtaining a pooled prior for inputs, $\tilde{q}^{[\theta]}(\theta)$, by inverting $\tilde{q}^{[\phi]}(\phi)$ backwards through the model. For values of ϕ that map to multiple points in θ , the density of those points is distributed in proportion to the prior density $q_\theta(\theta)$. Poole and Raftery (2000) showed that the proper way to arrive at $\tilde{q}^{[\theta]}(\theta)$, whether or not the model is invertible, is by the following formula

$$\tilde{q}^{[\theta]}(\theta) = \tilde{q}^{[\phi]}(\Phi(\theta)) \frac{q_\theta(\theta)}{q_\theta^i(\Phi(\theta))} \quad (4)$$

Implementation: SIR

Raftery et al. (1996) proposed a modification to the SIR algorithm to implement BYSM with geometric pooling so as to eliminate Borel's paradox. The modified SIR algorithm is carried out in the following five steps (Raftery and Poole 1997), which are reviewed here for completeness.

1. Draw a random sample of size M from the values of θ from its prior distribution $q_\theta(\theta)$. Denote the sample by $(\theta_1, \theta_2, \dots, \theta_M)$.
2. For each value of θ_k sampled in step 1, run the model to obtain the corresponding value of $\phi_k = \Phi(\theta_k)$.
3. Use nonparametric density estimation to obtain an estimate of $q_\theta^i(\phi)$, the resulting model-implied density of ϕ for $\{\phi_1, \phi_2, \dots, \phi_M\}$. Kernel density estimation with a Gaussian kernel has the advantage of being easily applied in higher dimensions (Silverman 1986, Scott 1992). The window width of the smoother was chosen by the normal reference rule (Scott 1992, p. 131).

4. Form importance sampling weights r_k using (5) with $\alpha = 0.5$ for geometric pooling.

$$r_k \propto \left(\frac{q_\phi(\Phi(\theta_k))}{q_\theta^i(\Phi(\theta_k))} \right)^{1-\alpha} L_\theta(\theta_k) L_\phi(\Phi(\theta_k)) \quad (5)$$

5. Sample m values, with replacement, from the discrete distribution of M values of (θ_k, ϕ_k) and sampling probabilities proportional to r_k .

When M/m is large, the result of SIR step 5 is an approximate sample from the geometrically pooled, post-model posterior distribution. It can be used to make inferences about quantities of interest, which may involve inputs or outputs or functions thereof.

Accounting for Correlations

To account for correlated model inputs analytically would require specifying a joint prior distribution for all inputs. For some situations this would be a reasonable task, assuming mathematically tractable PDFs were available to describe the joint distributions (e.g., bivariate normal distributions). In practice this will often be problematic as the number of inputs is large and joint relationships are not always easily defined. We used a nonparametric method that accounts for rank correlations between inputs rather than parametric specification of multivariate relationships. The method was developed for inducing correlations in random samples of model inputs for Latin Hypercube Sampling (Iman and Conover 1980). Iman and Conover (1982) described the correlation induction algorithm in detail, including numerical examples. A brief overview explaining how the method is implemented in BYSM follows.

Correlations are induced immediately following SIR step 1. In step 1, a large number (M) of input values are randomly generated for each of the P model inputs for which Bayesian priors are available. For convenience, the simulated values are arranged in a $M \times P$ data matrix \mathbf{D} . The columns of \mathbf{D} are random samples from the marginal priors of θ . A $P \times P$ positive definite target rank correlation matrix \mathbf{R} is specified. The restriction that \mathbf{R} be positive definite is due to the computation of the Cholesky decomposition of \mathbf{R} in the correlation induction algorithm. Correlations are induced by partially sorting the columns of \mathbf{D} to attain the target correlation structure. Since the algorithm only mixes values within the columns of \mathbf{D} , all marginal distributions are preserved. The rearranged data matrix \mathbf{D} will have a correlation structure identical to \mathbf{R} . Although the augmentation to SIR step 1 does not completely specify a joint distribution for $q_\theta(\theta)$, it does have the desirable effect of accounting for correlations between the inputs. SIR proceeds with the sample of M model input vectors that satisfy the target correlation structure.

Additional consideration for correlated inputs may be necessary in SIR step 4. Calculations of likelihoods involving inputs must account for the desired correlation structure. If data pairs (triplets, etc.) directly observed on the population of interest were available for inputs assumed *a priori* to be correlated, explicit formulas for their joint likelihood would be needed in SIR step 4 [Equation (5)]. If no directly observed

data were available for the correlated inputs, likelihood calculations involving these inputs would not be necessary.

Data

Having chosen to work with the model PnET-II, we identified a population of interest for which various direct and indirect sources of information about model inputs and outputs were obtainable. The mixed-species, broadleaved, deciduous forest of the USDA Forest Service Coweeta Hydrologic Laboratory in western North Carolina was chosen as the population of interest. PDFs for 29 PnET-II vegetation inputs for broadleaved, deciduous forests in the Eastern United States (Radtke et al. 2001) served as a source of indirect information for this population (Table 1). Indirect information relevant to soil and site-specific model quantities for Coweeta was compiled from published sources (Table 2) for the purpose of establishing data-based Bayesian priors for these model quantities. Although empirical observations were used in formulating priors, the indirect data themselves were not used in BYSM. Rather, the information conveyed by the indirect data was compiled as a set of PDFs to be used as Bayesian priors (Table 3).

Direct information pertaining to model inputs and outputs was compiled from observational studies conducted at Coweeta between 1987 and 1995 (Bolstad et al. 1998, Bolstad et al. 2001). The available data from Coweeta consisted of complete climate

records for the period of interest, average annual foliage, and wood production values observed at 16 study plots at Coweeta and the soil water holding capacity (WHC) measured at each plot. Foliage and wood biomass production data were summed and averaged for each field plot to obtain 16 observations of the mean aboveground net primary production (ANPP, g/m²/yr) over the duration of the study.

Prior Distributions and Correlations

A complete set of prior pdfs for PnET-II vegetation inputs was available (Table 1), but priors for soil and site-specific inputs and outputs were still needed. Similar methods to those employed by Radtke et al. (2001) were used to estimate priors for the soil and site-specific inputs and the model output ANPP. To estimate prior distributions, indirect information was compiled from published studies pertaining to populations similar to the forests at Coweeta (Table 2). Prior distribution PDFs were estimated from the indirect information. The goal for estimating priors was to make practical characterizations of the location, spread, and shape of the prior distributions. For some inputs, PDFs could be estimated from simple summary statistics of the compiled data sets, e.g., the mean and variance of the indirect observations for a normal prior PDF. For others it was necessary to make various assumptions or perform additional analyses. Descriptions of these assumptions and analyses follow.

Table 1. Distributions of PnET-II vegetation inputs for eastern deciduous forests of North America (Radtke et al. 2001).

| Input | Definition (units) | Family | Distribution |
|-------------------|--|-----------|---|
| AmaxA | Intercept of relationship between foliar N and max photosynthetic rate (Amax) | Normal | $\mu = -12.2, \sigma = 15.4$ |
| AmaxB | Slope of Amax versus N relationship; Amax ($\mu\text{mol CO}_2/\text{g leaf/s}$) | Normal | $\mu = 62.7, \sigma = 7.0$ |
| AmaxFrac | Daily Amax as a fraction of early morning instantaneous rate | Beta | $\alpha = 23.2, \beta = 7.30$ |
| BaseFolRespFrac | Respiration as a fraction of maximum photosynthesis | Beta | $\alpha = 6.0, \beta = 37.3$ |
| CfracBiomass | Carbon as a fraction of tissue mass | Weibull | $\beta = 0.494, \gamma = 35.4$ |
| DVPD1 | Coefficients for photosynthesis reduction due to vapor pressure deficit (VPD) | Normal | $\mu = -0.43, \sigma = 0.011$ |
| FolMassMax | Site specific maximum summer foliage biomass (g/m^2) | Lognormal | $\mu = 5.76, \sigma = 0.349$ |
| FolNCon | Foliar nitrogen (%) | Lognormal | $\mu = 0.74, \sigma = 0.26$ |
| FolRelGrowMax | Maximum relative growth rate for foliage (% /yr) | Uniform | $\alpha = 0.2, \beta = 0.5$ |
| GDDFolEnd | Growing degree days (GDD) at which foliar production ends | Normal | $\mu = 898, \sigma = 189$ |
| GDDFolStart | GDD at which foliar production begins | Normal | $\mu = 379, \sigma = 75$ |
| GDDWoodEnd | GDD at which wood production ends | Normal | $\mu = 1158, \sigma = 238$ |
| GDDWoodStart | GDD at which wood production begins | Normal | $\mu = 639, \sigma = 132$ |
| GrespFrac | Growth respiration, fraction of allocated carbon | Beta | $\alpha = 8.2, \beta = 23.0$ |
| HalfSat | Half saturation light intensity ($\mu\text{mol/m}^2/\text{s}$) | Weibull | $\beta = 299.9, \gamma = 1.87$ |
| k | Canopy light extinction constant | Normal | $\mu = 0.56, \sigma = 0.12$ |
| MinWoodFolRatio | Minimum ratio of carbon allocation to wood and foliage | Lognormal | $\mu = 0.46, \sigma = 0.42$ |
| PlantCReserveFrac | Fraction of plant carbon held in reserve after allocation to bud carbon | Uniform | $\alpha = 0.05, \beta = 0.95$ |
| PrecIntFrac | Fraction of precipitation intercepted and evaporated | Weibull | $\alpha = 0.11, \beta = 0.05, \gamma = 1.8$ |
| PsnTMin | Minimum temperature for photosynthesis ($^{\circ}\text{C}$) | Normal | $\mu = 0.68, \sigma = 0.64$ |
| PsnTOpt | Optimum temperature for photosynthesis ($^{\circ}\text{C}$) | Normal | $\mu = 22.2, \sigma = 0.33$ |
| RespQ10 | Q_{10} value for foliar respiration | Weibull | $\alpha = 1.9, \beta = 0.60, \gamma = 1.87$ |
| RootAllocB | Slope of relationship between foliar and root allocation | Normal | $\mu = 2.52, \sigma = 0.214$ |
| RootMRespFrac | Ratio of fine root maintenance respiration to fine root biomass production | Uniform | $\alpha = 0.5, \beta = 2.0$ |
| SenesceStart | Day of year after which leaf drop can occur | Normal | $\mu = 260, \sigma = 13$ |
| SLWDel | Change in SLW with accumulated foliar mass above ($\text{g/m}^2/\text{g}$) | Normal | $\mu = -0.155, \sigma = 0.014$ |
| SLWMax | Specific leaf weight (SLW) at top of canopy (g/m^2) | Normal | $\mu = 87.2, \sigma = 18.8$ |
| WoodMRespA | Wood maintenance respiration as a fraction of gross photosynthesis | Beta | $\alpha = 12.4, \beta = 99.8$ |
| WueConst | Coefficient in equation for water use efficiency (WUE) as a function of VPD | Normal | $\mu = 10.9, \sigma = 0.875$ |

Table 2. Sources and numbers of indirect observations (*n*) compiled from published literature for determining Bayesian prior PDFs for PnET-II soil and site-specific inputs and outputs of interest.

| Input/output | Units | Data source | <i>n</i> |
|---|-------------------------|--|----------|
| Aboveground Net Primary Production* | g/m ² /yr | Whittaker 1966, Whittaker et al. 1974, Crow 1978, Aber et al. 1993, and Fassnacht and Gower 1997 | 34 |
| Soil Water Release Parameter (<i>f</i>) | n/a | n/a | — |
| FastFlowFrac | cm/cm | Woodruff and Hewlett 1970 | 14 |
| SoilMoistFact | n/a | n/a | — |
| SoilRespA (intercept) | g/m ² /mo | Reiners 1968, Edwards 1975, and Peterjohn et al. 1994 | >156 |
| SoilRespB (slope) | g/m ² /mo/°C | Reiners 1968, Edwards 1975, and Peterjohn et al. 1994 | >156 |
| WHC [†] | cm | USDA Natural Resources Conservation Service 1994 | 21 |

* Model output (ANPP).

† Soil available water capacity, no account for rooting depth.

For the PnET-II inputs *f* and SoilMoistFact no empirically observed values were found in published literature. Given this scarcity of information, extreme values were postulated and uniform distributions between them were assumed (Table 3).

Bootstrap sampling was used in combination with regression analyses to estimate prior distributions for the model inputs SoilRespA and SoilRespB. Data obtained from figures published by Reiners (1968), Edwards (1975), and Peterjohn et al. (1994) were the primary sources of information. First, 234 observed soil CO₂ efflux (i.e., respiration, g C/m²/day) and mean daily soil temperature (DTsoil, °C) data were used to fit a daily CO₂ soil efflux submodel

$$\ln(\text{Soil Respiration}) = -0.4489 + 0.106DT_{\text{soil}} \quad (6)$$

The root mean-squared error (RMSE) for (6) was 0.39. Next, a regression of DTsoil versus average daily air temperature (DTair, °C) was fitted to 156 data pairs of Peterjohn et al. (1994), with a resulting RMSE = 1.93 °C.

Third, a simulation was carried out to account for the combined errors when using predicted soil temperature as a dependent variable in fitting (6). For the 156 DTair observations reported by Peterjohn et al. (1994), simulated DTsoil data were generated by the fitted model DTsoil = 5.1 + 0.61DTair plus a random variable $\epsilon \sim \text{Normal}(0, \sigma = 1.93)$. Soil respiration data (log scale) were generated for the DTsoil random values from (6) plus an additional random component $\sim \text{Normal}(0, 0.39)$. One-hundred bootstrap samples (Efron and Tibshirani 1993) were drawn from the simulated 156 data pairs. A model of the form $\ln(\text{Soil Respiration}) = b_0 + b_1DT_{\text{air}}$ was fitted for each bootstrap sample. Exponentiation of the model and multiplying by 31 gave the monthly soil respiration model used in PnET-II

$$\text{Soil Respiration (gC / m}^2 / \text{mo}) = \text{SoilRespA} \times \exp^{b_1DT_{\text{air}}} \quad (7)$$

where $\text{SoilRespA} = 31\exp(b_0)$ and $\text{SoilRespB} = b_1$. The constant 31 is used to convert daily soil respiration values to a monthly scale. [Note: results of Kicklighter et al. (1994) show that no appreciable variability is introduced when converting daily values to a monthly scale.] Bootstrap estimates of the mean and standard deviation of SoilRespA and SoilRespB were computed (Table 3). Inspection of the bootstrap sample regression coefficients showed nearly symmetric unimodal distributions so a normal PDF was chosen to characterize their distributions.

For some model inputs data were collected in pairs that made it possible to estimate the correlation between inputs. Table 4 lists empirical correlation coefficients observed by Radtke et al. (2001) for pairs of PnET-II inputs that describe vegetation characteristics. The correlation coefficient estimated from the bootstrap sample for the model parameters SoilRespA and SoilRespB is also listed in Table 4. The Table 4 correlations were specified in **R** in the correlation induction algorithm previously described. The purpose of this step was to account for correlations between model inputs in specifying $q_{\theta}(\theta)$.

Fixed Inputs

In addition to input parameters that describe vegetation, soil, and site-specific traits of the population to be modeled, PnET-II requires input values for initial conditions and climate variables during the simulation. Snow cover at the start of the simulation (January 15, 1987) was set at zero based on snow cover records from nearby Asheville, NC on that date [Source: National Climate Data Center online archive (ac-

Table 3. PnET-II soil and site-specific prior PDFs for inputs and outputs pertaining to Coweeta.

| Input/output | Family | Estimation | Distribution | KS test <i>P</i> -value |
|------------------|-----------|-----------------------|--------------------------------|-------------------------|
| ANPP* | Lognormal | Summary statistics | $\mu = 6.80, \sigma = 0.311$ | 0.77 |
| <i>f</i> | Uniform | Assumption | $\alpha = 0.02, \beta = 0.06$ | |
| FastFlowFrac | Beta | Summary statistics | $\alpha = 4.19, \beta = 60.0$ | 0.72 |
| SoilMoistFact | Uniform | Assumption | $\alpha = -1, \beta = 1$ | |
| SoilRespA | Normal | Regression, bootstrap | $\mu = 27.5, \sigma = 1.71$ | |
| SoilRespB | Normal | Regression, bootstrap | $\mu = 0.068, \sigma = 0.0036$ | |
| WHC [†] | Normal | Summary statistics | $\mu = 24.7, \sigma = 5.2$ | 0.06 |

* Model output.

† Soil available water capacity, no account for rooting depth.

Table 4. Correlation coefficients and number of indirect observations (n) for PnET-II input pairs.

| Variable pair | Correlation | n |
|----------------------|-------------|-----|
| AmaxA, AmaxB* | -0.97 | 28 |
| FolNCon, FolMassMax* | -0.49 | 31 |
| PsnTMin, PsnTOpt* | 0.67 | 104 |
| SLWMax, SLWDel* | 0.73 | 15 |
| SoilRespA, SoilRespB | -0.66 | 100 |

* From Radtke et al. (2001).

cessed 5/01): <http://www.ncdc.noaa.gov/>. Soil available water was assumed to be equal to water holding capacity (WHC), assuming saturated soil conditions in mid-January. Monthly averages for PnET-II climate inputs were tabulated from climate station 1 at Ceweeta (Table 5): daytime high (T_{max}) and nighttime low (T_{min}) temperatures (°C); photosynthetically active flux density (PPFD, $\mu\text{mol}/\text{m}^2/\text{sec}$); and precipitation (Precip, cm). Unlike the input parameters needed to conduct PnET-II simulations, T_{min} , T_{max} , PPFD, and Precip were not considered parameters of the population of interest; instead, we considered them external variables that act on the ecosystem. BYSM does not distinguish between input variables and input parameters so it would have been possible to develop priors for the climate inputs and use observed climate data to compute likelihoods, proceeding with the BYSM estimation of posteriors for these quantities. However, having seen no need to estimate Bayesian posterior distributions for these known inputs, we treated them as fixed, thereby removing them from the BYSM uncertainty analysis.

Experimental Scenarios

Two scenarios for specifying prior correlations for inputs were postulated for testing the study hypotheses. Scenario 1 was the “no-correlation” scenario, where all inputs were assumed to be independent. Scenario 2 specified the known prior correlations listed in Table 4. By testing whether or not posterior correlations were present under the no-correlation scenario, evidence could be gathered to assess the utility of explicitly accounting for correlations in BYSM priors. For scenario 1, a $P \times P$ identity matrix was specified as the target correlation matrix. For scenario 2, the target correlation matrix included off-diagonal elements listed in Table 4.

Results

BYSM was carried out with $M = 100,000$ model vectors generated at SIR step 1 and $m = 2000$ model vectors selected (with replacement) at SIR step 5. The value of M was chosen to be as large as possible given a practical constraint that the analysis would require under 8 hr of execution time on a desktop computer. For BYSM under experimental scenario 1, the number of unique model vectors (m^*) in the SIR Step 5 posterior sample was $m^* = 1,292$. BYSM under scenario 2 results were similar with $m^* = 1,253$. It followed that the posterior sample sizes were sufficiently large to provide reasonable estimates of the posterior distributions of interest.

Input Correlations

Posterior distributions were examined for the input pairs listed in Table 4 for both experimental scenarios.

Table 5. Climate inputs for PnET-II simulations of Ceweeta forests. Data averaged from climate station observations taken from 1987–1995 at Ceweeta.

| Month | T_{min}(°C)..... | T_{max} | Precip (cm) | PPFD ($\mu\text{mol}/\text{m}^2/\text{sec}$) |
|-------|-----------------------------|-----------|----------------|---|
| 1 | -1.1 | 8.1 | 20.9 | 572 |
| 2 | 0.0 | 9.4 | 21.7 | 739 |
| 3 | 3.3 | 13.5 | 23.6 | 863 |
| 4 | 7.0 | 17.7 | 14.1 | 1021 |
| 5 | 11.2 | 21.7 | 13.4 | 997 |
| 6 | 15.1 | 25.1 | 17.5 | 920 |
| 7 | 17.2 | 27.2 | 15.9 | 939 |
| 8 | 16.8 | 26.2 | 18.7 | 886 |
| 9 | 13.7 | 22.9 | 17.4 | 816 |
| 10 | 7.5 | 18.2 | 15.5 | 885 |
| 11 | 3.5 | 13.3 | 19.4 | 730 |
| 12 | -0.1 | 8.5 | 17.4 | 587 |

When BYSM was conducted under scenario 2, the prior correlations were generally reflected in the posterior sample (Table 6). Pairwise rank correlation coefficients (r) in Table 6 were tested one at a time against null hypotheses in the form $H_o: r - \rho_o = 0$, where empirical ρ_o values and their corresponding sample sizes (n) from Table 4 were the basis for comparison. Hypotheses were tested based on the Fisher transformation to normality, using the test statistic $Z(r - \rho_o) = \tanh^{-1}(r) - \tanh^{-1}(\rho_o)$ to transform the sample rank correlation coefficient differences, and assuming a mean of zero and variance of $(m - 3)^{-1} + (n - 3)^{-1}$ under H_o (Fisher 1970). Under scenario 1, the null hypotheses were rejected for all five posterior correlations (all $P < 0.01$). Under scenario 2, the null hypotheses could not be rejected for any of the five posterior correlations (all $P > 0.3$).

Accounting for correlations between the model inputs listed in Table 4 had some effect on inducing correlations between other pairs of inputs. We computed Spearman rank correlation coefficients (r) for all 595 pairwise relationships between the 35 model inputs examined. The mean absolute values of the computed correlation coefficients were small, 0.029 for scenario 1 and 0.037 for scenario 2. Choosing any pairwise $|r| > 0.058$ as a threshold for significance ($\alpha = 0.01$ based on Fisher's transformation) when compared to the null hypothesis of no correlation, the number of significant pairwise correlations observed, n_{corr} , was tallied for each scenario. The five input pairs listed in Table 4 were omitted from calculations of n_{corr} since its intended use was to determine whether specification of prior correlations might affect the distributions of model quantities not directly involved with the prior correlation. For scenario 1 $n_{corr} = 63$ was observed, while a larger number of significant pairwise correlations was observed under scenario 2, $n_{corr} = 89$.

In addition to calculating the number of significant posterior pairwise correlations, we examined pairs of

Table 6. BYSM posterior sample Spearman rank correlation coefficients comparing BYSM for scenario 1 (independent input priors) and scenario 2 (correlated inputs from Table 4).

| Variable pair | Scenario 1 | Scenario 2 |
|----------------------|------------|------------|
| AmaxA, AmaxB | -0.02 | -0.96 |
| FolNCon, FolMassMax | 0.04 | -0.46 |
| PsnTMin, PsnTOpt | -0.05 | 0.64 |
| SLWMax, SLWDel | 0.00 | 0.69 |
| SoilRespA, SoilRespB | -0.03 | -0.64 |

Table 7. BYSM posterior rank correlation coefficients for PnET-II input pairs exhibiting greatest posterior correlation under experimental scenarios 1 (independent priors) and 2 (correlated priors). Listed *P* values are computed from pairwise null hypotheses of the same posterior correlation under both scenarios.

| Input pair | Scenario 1 | Scenario 2 | <i>P</i> value |
|--------------------------|------------|------------|----------------|
| FolNCon, HalfSat | 0.37 | 0.47 | 0.01 |
| AMaxFrac, HalfSat | 0.26 | 0.27 | 0.81 |
| BaseFolRespFrac, HalfSat | -0.23 | -0.27 | 0.34 |
| SLWMax, HalfSat | 0.21 | 0.23 | 0.64 |
| AMaxA, HalfSat | 0.19 | 0.10 | 0.04 |
| FolNCon, SLWMax | -0.18 | -0.10 | 0.07 |
| AMaxB, HalfSat | 0.20 | -0.07 | <0.01 |
| FolNCon, k | 0.12 | 0.14 | 0.65 |
| BaseFolRespFrac, FolNCon | 0.13 | 0.13 | 1 |
| FolMassMax, HalfSat | 0.00 | -0.26 | <0.01 |

model inputs that exhibited the greatest pairwise rank correlations in the BYSM posterior sample (Table 7). The input pairs shown in Table 7 were selected based on having the largest sums of their absolute rank correlation coefficients compared to all other input pairs. For most of the pairs shown in Table 7, the magnitude and sign of their rank correlation are not significantly different between experimental scenarios (i.e., $P \geq 0.1$). For a few input pairs, the magnitude and/or sign of their rank correlation are distinctly different between the two scenarios (i.e., $P \leq 0.01$). For a few others, only subjective determination can be made as to whether the magnitudes are significantly different (i.e., $0.01 < P < 0.1$).

Prior to conducting the investigation, we were not aware of any known relationship between the model inputs HalfSat and FolNCon; however, BYSM posterior results indicated a moderate correlation between these two parameters (Table 7). A closer examination of results presented by Sullivan et al. (1996) was made to obtain further evidence to support or contradict this result. HalfSat values derived by Radtke et al. (2001) were paired with leaf nitrogen values from the same

data source (Sullivan et al. 1996). A total of 10 data pairs were obtained, with a sample correlation of 0.57 (Figure 1). A null hypothesis of no correlation between leaf nitrogen and HalfSat was tested against a one-tailed alternative, using these 10 data pairs to test the hypothesis. The test showed evidence ($P = 0.04$) to reject the null hypothesis in support of the conclusion of positive correlation between HalfSat and FolNCon, which was initially indicated by the BYSM posterior sample.

Marginal Distributions

In general, uncertainty assessments for process-based models may be concerned with any model inputs or outputs of interest. For studies intended to assess uncertainty in existing model predictions, interest would lie mainly in the posterior distributions of model outputs. For studies intended to improve prediction accuracy for future applications, posterior distributions of model inputs would also be of interest. In the BYSM analyses conducted here, accounting for correlated model inputs did not affect the posterior marginal distribution of predicted ANPP as compared to BYSM analysis ignoring prior correlations. The ANPP posterior means for scenarios 1 and 2 were both 894 g/m²/yr, and the standard deviations were 40.1 and 40.5 g/m²/yr, respectively. There was no detectable difference between these alternative posterior distributions ($P = 0.46$), based on results of a two-sample Kolmogorov-Smirnov (KS) test (Darling 1957, Lindgren 1993 p. 485).

For the 35 model inputs, posterior means and standard deviations were generally similar, regardless of the specification of independent or correlated input priors; however, KS tests showed evidence of differences between the posterior distributions of some inputs, depending on whether or not input correlations were specified *a priori* (Table 8). Differences indicated by the KS tests were generally due to moderate or slight deviations in the shapes of the distributions between scenarios 1 and 2, such as those illustrated in Figure 2.

Discussion

Input Correlations

The correlation induction algorithm demonstrated here is an enhancement to BYSM for inducing prior correlations without explicitly formulating joint PDFs. The technique is useful when correlations are known to exist *a priori* between pairs of model inputs, such as was the case for several pairs of inputs for the model PnET-II here (Table 4). For the pairs of inputs examined, none of the correlations in the posterior sample could be distinguished from the corresponding hypothesized (i.e., prior) correlations. Conversely, under the prior assumption of independence, all of the posterior correlations were distinctly different from the corresponding hypothesized values. These results indicate that the algorithm for inducing prior correlations achieved its intended purpose. In BYSM analyses where there is some prior information about correlations between pairs of model inputs, the method demonstrated here provides a tool for accounting for them. The technique would be useful in situations where explicit formulation of joint PDFs was difficult, for example in cases where the joint distribution was not known or was

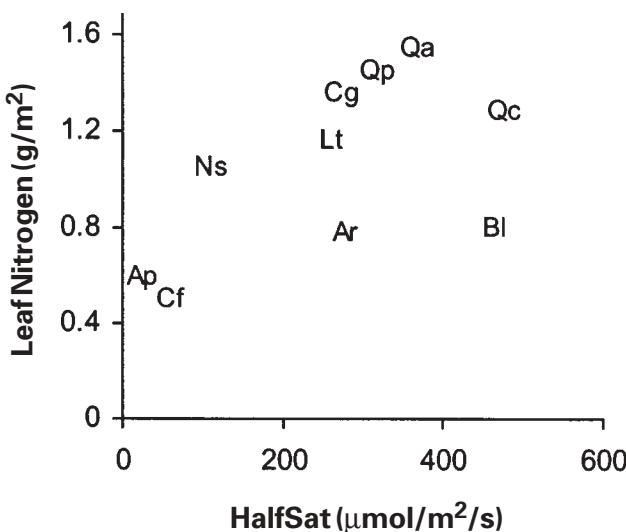


Figure 1. Leaf nitrogen per unit area versus half saturation light intensity (HalfSat) for ten species studied by Sullivan et al. (1996). Ap = Acer pensylvanicum, Ar = A. rubrum, Bl = Betula lenta, Cf = Cornus florida, Cg = Carya glabra, Lt = Liriodendron tulipifera, Ns = Nyssa sylvatica, Qa = Quercus alba, Qc = Q. cocinea, Op = Q. prinus.

Table 8. BYSM posterior summary statistics from scenarios 1 (independent priors) and 2 (correlated priors) for PnET-II inputs, with P -values from two-sample KS tests comparing the alternative posterior distributions. KS tests for inputs not listed here resulted in P -values ≥ 0.1 .

| Input | Scenario 1 | | Scenario 2 | | P |
|-----------------|------------|-------|------------|-------|--------|
| | Mean | SD | Mean | SD | |
| FolMassMax | 340 | 120 | 352 | 117 | < 0.01 |
| GDDFolEnd | 910 | 179 | 896 | 184 | < 0.01 |
| SLWDel | 0.16 | 0.01 | 0.15 | 0.01 | < 0.01 |
| SLWMax | 86 | 19 | 84 | 18 | 0.01 |
| PrecIntFrac | 0.15 | 0.03 | 0.15 | 0.03 | 0.01 |
| AMaxB | 62.3 | 7.0 | 63.0 | 7.1 | 0.01 |
| SoilMoistFact | -0.02 | 0.59 | 0.01 | 0.57 | 0.03 |
| GRespFrac | 0.27 | 0.08 | 0.27 | 0.08 | 0.03 |
| AMaxA | -12.9 | 14.3 | -12.8 | 15.7 | 0.04 |
| DVPD1 | -0.04 | 0.01 | -0.04 | 0.01 | 0.06 |
| SoilRespB | 0.068 | 0.004 | 0.068 | 0.004 | 0.06 |
| MinWoodFolRatio | 1.79 | 0.78 | 1.74 | 0.74 | 0.07 |
| AMaxFrac | 0.76 | 0.08 | 0.75 | 0.07 | 0.08 |

not tractable. The technique would be particularly useful in situations where model inputs were correlated with numerous other inputs, as all pairwise correlations could be specified in the matrix \mathbf{R} .

A weakness of the method is that it cannot be used by itself to account for correlations between model inputs for which direct data were observed. The correlation induction algorithm only accounts for correlations in the prior distribution, i.e., at SIR step 1, where values are drawn from $q_{\theta}(\theta)$. Calculations involving $L_{\theta}(\theta)$, for inputs on which direct observations were made would require explicit formulation of a joint PDF to derive the corresponding likelihood function. For example, denoting a pair of correlated model inputs X and Y , and assuming some prior correlation ρ , the correlation induction algorithm would be used at SIR step 1 to induce ρ . At SIR step 4, it would be necessary to compute likelihoods for each (X, Y) pair generated in SIR step 1 (denoted θ_x, θ_y). This would require making some assumption about their joint PDF. If X and Y were assumed to be joint-normally distributed, a bivariate Gaussian likelihood function would be used to compute the likelihood of each SIR step 1 (θ_x, θ_y) pair (Lindgren 1993, p. 222, 418).

Such calculations may become considerably more complicated when input pairs do not conform to a simple joint distribution such as the bivariate normal distribution. Examination of Tables 1 and 4 reveal that 4 of the 5 correlated input pairs could be assumed to follow joint-normal prior distributions, and the fifth pair (FolNCon, FolMassMax) could be assumed to follow a joint-lognormal distribution. Had direct

observations been available for any or all of these inputs, computation of likelihoods would have been possible.

It would require considerable effort for an investigator to directly observe data for many of the model inputs listed in Table 4. Here, we had no direct information about any of them. Given the nature of process-based model inputs and the difficulty of obtaining direct observations of them, it seems reasonable that investigators would most often have indirect information available about correlated model inputs. Directly observed data would seldom be available for computing likelihoods for correlated model inputs. From this principle, it follows that joint-likelihood calculations will seldom be a practical concern for conducting BYSM analyses of process-based models like PnET-II. The need to specify prior correlations will be far more common, so nonparametric methods like the one implemented here should have considerable utility.

To date, little work has been done to address the issue of correlated inputs in BYSM. Guan (2000) demonstrated the utility of the method of Iman and Conover (1982) to problems involving evaluation of process-based models used in forestry and suggested that the technique could be applied to BYSM. Green et al. (1999) suggested that the BYSM posteriors could characterize correlations between model inputs, even under the prior assumption of independence. While possible, the results presented here do not support this as a necessary outcome of BYSM. Likelihood data were used for only one model input here (WHC) and one model output (ANPP). Given the paucity of data used to calculate likelihoods here, it is not entirely surprising that BYSM did not produce posterior correlations to match Table 4 under the prior assumption of independence. Had detailed observations of more inputs been incorporated into the analysis, the likelihood calculations might have produced the target correlations in the posterior distributions.

In order for this to occur, the functions used to compute likelihoods should allow a mechanism for input correlations to be accounted for. A bivariate normal likelihood function, for example, provides such a mechanism, so that if observed (X, Y) data pairs used in its calculations were correlated, then the BYSM posterior distribution should reflect that correlation. However, if one had no prior belief

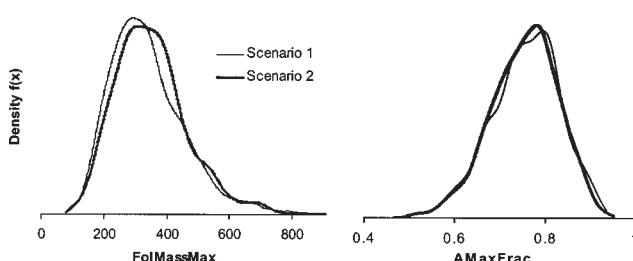


Figure 2. Comparison of BYSM posterior marginal distribution for the PnET-II inputs FolMassMax and AmaxFrac based on a prior assumption of independent inputs (Scenario 1) versus the prior assumption of correlations from Table 4 (Scenario 2).

that X and Y were correlated, it would be reasonable to formulate their likelihoods as the product of two independent normal likelihood functions. Thus, it becomes apparent that simply including direct observations of X and Y in the BYSM might not produce any posterior correlation between X and Y . In either case of having available direct observations or not, it would seem prudent to account for correlations as explicitly as possible in the specification of prior distributions and likelihoods.

Although the BYSM analysis conducted here did not generate the hypothesized correlations for targeted inputs of its own accord, significant (nonzero) posterior correlations were observed for nontargeted model inputs. The numbers of significant correlations were small compared to the findings of Green et al. (1999), who observed significant relationships among 44% of all possible input pairs tested at the $\alpha = 0.01$ level for the PIPESTEM model (Valentine 1998). The average magnitude of the absolute values of posterior correlations was also smaller here, around 0.03, compared to Green et al. (1999), who observed a value of 0.14. Their posterior sample size was considerably larger ($m = 5000$), and they tested fewer pairwise correlations (276), thus the probability of spurious nonzero correlations in their posterior sample should have been relatively small.

The possibility of spurious nonzero correlations should be considered, especially since pairwise tests of significance were used to test against the null hypotheses of independence. One would expect a Type I error rate of 1 in 100 ($\alpha = 0.01$), which corresponds to roughly 6 Type I errors when conducting 595 pairwise tests, as was done here. The same number of Type I misclassifications would be expected under either scenario 1 or 2, so the comparison between the two n_{corr} values should not be affected by this problem. One factor that may help to minimize Type I errors in testing posterior correlations is the use of the identity matrix for \mathbf{R} when generating the SIR step 1 sample. Specifying \mathbf{R} as the identity matrix effectively removes any nonzero correlations that may have occurred by random chance in generating the SIR step 1 values.

Regardless of whether input correlations were known to exist *a priori*, the BYSM posterior sample provides updated information about the joint distributions of any model inputs of interest. The nonzero values of n_{corr} observed under both experimental scenarios indicate that prior beliefs about independence of inputs can be re-examined for possible updating *a posteriori*. Information about such relationships may be useful for a variety of applications such as subsequent uncertainty assessments or sensitivity analysis (Elston 1992, Guan 2000). Posterior relationships may also provide information about actual relationships in the system being modeled. Such results may form the basis for hypotheses to be tested in future research, such as the hypothesis that HalfSat and FolNCon are positively correlated in broadleaved, deciduous canopies. Given the prominence of HalfSat and FolNCon in the processes that control canopy carbon balance, such a hypothesis may help model developers to verify that the algorithms they've designed to mimic these processes are working adequately.

Output Correlations

In addition to learning about correlations between model inputs, it is possible to use the BYSM posterior sample to update information regarding relationships between model outputs. For example, here we only considered the aggregated model output ANPP. PnET-II gives predictions of the components of ANPP, foliage and wood production, as well. Examining the foliage and wood production data pairs that comprised the BYSM posterior sample should provide information about their marginal and joint distributions. A more proactive approach than that described here would be to specify a prior joint distribution for foliage and wood production, then account for their joint distribution throughout the SIR procedure. Based on published foliage and wood production values from forests in eastern North America (e.g., Whittaker 1966, Whittaker et al. 1974, Crow 1978, Aber et al. 1993, Yin 1993, and Fassnacht and Gower 1997, Martin and Aber 1997) a data-based joint prior distribution could be established for wood and foliage production. Assuming that a bivariate normal or lognormal distribution describes the outputs' joint distribution adequately, calculations for $L_{\phi}(\phi)$ would be straightforward based on the component measurements of foliage and wood production observed directly on the population at Coweeta. The resulting BYSM posterior sample would portray the joint distribution of the model outputs, i.e., foliage and wood production, in a way that explicitly accounts for their correlation structure throughout the analysis. Performing such a procedure follows directly from the established BYSM technique and does not require additional implementation of the nonparametric correlation induction algorithm used here.

Marginal Distributions

For the BYSM analyses performed here, accounting for versus ignoring input correlations had little practical effect on the marginal posterior distributions of any individual model quantities. A possible exception was the result that the shapes of a few model input distributions changed perceptibly when prior correlations were accounted for. While this result cannot be generalized to all BYSN analyses, it demonstrates that correlation structures in modeling applications can vary significantly without affecting individual marginal distributions. Given the paucity of direct data used to compute likelihoods here, this result is not surprising. For BYSM analyses that involve many correlated inputs and outputs, and where more direct observations are incorporated into the analyses, one would expect that accounting for correlations could have significant effects on marginal distributions of any number of individual model quantities.

Fixed Inputs

Climate inputs were not subjected to the same uncertainty analysis as the other model inputs in this study. Here, there was very little uncertainty associated with the climate inputs since they were observed continuously over the duration of the study at Coweeta. It may be possible to account for the inherent variability in the climate inputs using BYSM; however, doing so would require substantial additional effort. This study examined inputs known *a priori* to exhibit simple

pairwise correlations. In comparison, climate inputs involve complex interrelationships that change over time within and between years. Radtke (1999) addressed this issue by developing regression models of long-term annual climate patterns for the PnET-II inputs T_{min} , T_{max} , PPF , and *Precip* for eastern North America, including Coweeta. These models generated 12 monthly climate values to be used as a single year's input to PnET-II, based on a single predictor, average annual temperature, precipitation, or PPFD.

While such models can be used to describe and simplify the complex relationships between climate inputs, they effectively modify the model being studied, which is generally considered an undesirable practice when assessing model uncertainties. Process-based models like PnET-II are designed to accurately represent system processes at levels of spatial, temporal and structural resolution appropriate for model's intended purpose. The analyses described here do not account for possible inaccuracies in model structure. Further research will be needed to account for complex interrelationships between model climate inputs in BYSM, especially if the ultimate goal is to incorporate direct data and likelihood calculations into the analyses. Accounting for possible errors in model structure within the framework of BYSM is another subject for possible future research.

Conclusions

As the use of process-based forest ecosystem computer models continues to increase, so does the need for methods to accurately assess model prediction uncertainties. BYSM is one such method. It provides a means of estimating Bayesian posterior distributions for any model quantities of interest. The posterior distribution incorporates information from a variety of sources including prior knowledge, data, and the model itself. As such, its inference base is stronger than model evaluation techniques that incorporate only one or two of these sources of information. Up to the present, BYSM analyses have not typically accounted for correlated model inputs, even though failing to account for such correlations may have lead to significant errors in evaluating model uncertainties (Iman and Conover 1982, Guan 2000).

The research presented here shows how prior knowledge about correlations between model inputs can be accounted for in BYSM. For five pairs of model inputs examined here, ignoring prior correlations resulted in an unsatisfactory representation of pairwise correlation in the posterior distribution. For many other pairs of model inputs, even though no prior correlations were specified, the posterior samples indicated evidence of pairwise correlations. We conclude that, if correlations are known to exist *a priori*, efforts should be made to explicitly account for them in BYSM analyses; however, posterior distributions may provide useful updated information about correlated model inputs, even when no prior knowledge about their correlation existed.

The technique shown here is subject to some limitations, namely that it does not completely specify the joint Bayesian prior distributions, only sets of pairwise rank correlations. It was shown that, for simple cases such as bivariate normal

distributions, complete specification of joint PDFs would be practical; however, this would only be necessary if likelihood calculations for correlated inputs were needed.

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