Statistical Inference for Food Webs with Emphasis on Ecological Networks via Bayesian Melding

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SUMMARY

Quantifying activities in a food web or ecological network, and related aspects of dependence, has largely been either descriptive or deterministic. Although schemes exist for assessing the reliability of such quantification, many are far from being statistical in nature. Statistical modeling approaches are explored, with a focus on the ecosystem aspects of a food web. By employing Bayesian melding, we provide a new statistical inferential approach for understanding ecological networks in the context of mass balance. Our approach embodies the traditional deterministic views on network relations, yet it is developed on the basis of proper statistical inference that allows the estimation of physical quantities and probabilistic assessment of the estimation. We describe our approach, and illustrate it with a mass balance dataset. The practical advantage of our approach is a more realistic understanding of the network by incorporating natural measurement variability into deterministic beliefs about the relationships among measurements. The resulting inference thus forms a more honest representation of the true state of nature, and provides a formal assessment of balance before data are passed on to later stages of an ecological network analysis (ENA). We also demonstrate that general Bayesian inference for ENA can yield new ecological insight that may not be available through standard classical inference.

KEY WORDS: Bayesian melding; deterministic models; ecological networks; food webs; statistical inference; statistical modeling

1 INTRODUCTION

The term food web loosely refers to a complex network of species. Its complexity can be compounded by factors such as inflow and outflow of material and energy through the system, and the interdependence among these factors and predatory behavior. Aspects such as how crucial is the existence of one species to sustain the food web are vital in food web research.

There are two main types of focuses when studying food webs. First, in the trophic context, the hierarchy of the feeding or predatory structure is the basis of the analysis. Thus, it involving data that pertain to the presence or absence of a link between a pair of species, and the direction of the link if present. Trophic food web analyses are largely non-model-based, but involve using the identification of predator and prey species to quantify network qualities such as inter-species connectance, species dominance, a species’ relative importance to the network, etc., thereby allowing systematic identification of species groupings such as trophic levels and compartments (e.g. Frank, 1995; Johnson et al., 2001; Krause et al., 2003, Vázquez et al., 2007).

Focus can also be placed on the ecosystem or whole-system level, where physical and chemical variables such as material and energy transfer and dissipation are considered alongside trophic aspects of the web, although these variables take center stage. Thus, whole-system analyses are based on specific numerical variables associated with the links. This whole-system approach is often known as ecological network analysis (ENA), on which methodological advances and open questions continue to emerge (e.g. Belgrano et al., 2005; Fath et al., 2007; Ulanowicz, 2004). Unlike trophic analyses, a key feature of ENA is the use of a deterministic mass balance model
that describes interdependence among all key compartments in the system, derived based on thermodynamic theory that constrains inter-compartmental transfer in a certain manner. Given such a model, all quantities must be balanced accordingly before any conclusions can be drawn about the ecosystem’s characteristics. Some recent publications on ecosystem balance modeling appear in the form of an “instructions manual” or “handbook” that accompanies numerical software created to implement certain models and solve for unobserved quantities by “maximizing balance.” (In essence, quantities that are unobserved are deduced — hence, “solved for” — from the observed through the balance model. This idea will be elaborated upon in Section 2.) For example, Eco-path with Ecosim (EwE) is a software attributable to Christensen and Pauly (1992) and Pauly et al. (2000), and EcoNetwrk, to a long list of ongoing works (thus, not explicitly referenced here) by Ulanowicz and his colleagues; both programs are widely used. For more general ENA techniques, Ulanowicz appears as co-author on many papers cited in this section, and has published prolifically on the topic.

As is the case for many areas of active research, quantitative food web analysis methodologies are subject to improvement. Some major criticisms targeting the current status of ENA appear in Dame and Christian (2006). These authors suggest that (a) the fundamental assumption of linear balance and the rigidity of deterministic models in ENA remain a concern; (b) ENA ignores much of the information available on the sources of variability in the observed quantities, whose effects on the deduced quantities are largely unexamined; (c) few systematic techniques exist for objectively assessing and validating ENA, as alternative methods are structurally different; (d) standard ENA depicts a snapshot in time, so that monitoring the network spatially or temporally is difficult, and predicting future quantities is virtually impossible; and (e) although Ecosim and Ecospace (an extension of EwE) allow prediction by turning the Ecopath balance model into a dynamical simulation model (also physical-theoretic), “[a]ny uncertainty in the Ecopath base model is potentially compounded as it is used up the hierarchy in complexity from Ecosim to Ecospace.” We also note that existing efforts to monitor networks over space or time based on non-dynamical models are often crude, appearing in the form of qualitative comparisons of externally derived indices (e.g. Bundy and Fanning, 2005). Statistically speaking, point (c) above ultimately pertains to having no obvious way to assess how reliable is the so-called “balance solution” for describing the underlying ecosystem. Indeed, little stochastic modeling exists for ENA apart from basic empirical experimentation with sensitivity (e.g. Bundy, 2005; Essington, 2007).

Some of Dame and Christian’s criticisms appear to be applicable also to trophic food web analyses. Point (b) above addresses the lack of stochasticity in the analysis, which is often the case for trophic studies, too. Again, (c) may be interpreted as a statistical issue, and the same lack of assessment scheme is true for most trophic analysis techniques. Vázquez et al. (2007) and Krause et al. (2003) assess significance of identified groupings by what is essentially a permutation test, where links are randomly redistributed among species and compartments reassessed. While it appears to be proper non-parametric statistical inference, variability of the observed links are not built into the analysis in the first place, which, if statistically modeled, could have been utilized to (perhaps drastically) improve the power of the significance test. Solow (2005) notes that, in
general, a bigger emphasis on statistical inference is necessary when analyzing food webs. On a broader scope yet, McMahon et al. (2001) advocate continuing in the interdisciplinary direction in order to improve our understanding of complex food web or ecological network structures.

Thus, food web methodologies are expected to show further advancement in different directions in years to come. We believe that one such direction is the honest acknowledgment of natural variability that is inherent in the measurements used to produce the quantitative analysis, but without going as far as to say, “the analysis is not very meaningful in the face of variability.” Specifically, it appears natural to integrate statistical modeling techniques to incorporate this variability directly into the analysis phase, instead of using statistical tools as a post-analysis assessment. Little work, if any, currently exists in this regard, in either the trophic or whole-system context. As data types are structurally different between the two, it may be sensible to develop separate statistical modeling methodologies according to the data types. For trophic data, Chiu and Westveld (in progress) are currently developing an adaptation of statistical modeling of social networks (SNs) (Hoff et al., 2002; Ward and Hoff, 2007; Westveld, 2007). This approach is unlike conventional social network analysis techniques that are largely descriptive in nature. In a statistical SN model, sender-receiver links appear as correlated random effects that may be expressed as functions of latent factors which underlie the interaction mechanism. Moreover, longitudinal SN models incorporate temporal dependence of links, in addition to covariates that help to explain the interactions. Taking prey as senders and predators as receivers, this type of modeling (i) enables proper inference for longitudinal or pointwise estimation / prediction of species behavior, including predation activity level and preference, without relying on externally defined descriptive indices; and (ii) accounts for the different sources of data and other relevant factors, including whole-system level variables, by expressing them as covariates. Both are achievable simultaneously through a single model. This methodology not only addresses some aforementioned concerns about food web techniques, but it can also add an extra dimension to trophic analyses by naturally incorporating whole-system level variables.

However, the statistical SN approach retains a trophic emphasis, in that no physical theory among the whole-system level variables is utilized in the model. This is separately addressed in the remainder of our article, where we describe and illustrate our new approach that integrates statistical modeling with ENA balance modeling via Bayesian melding (Poole and Raftery, 2000). The complexity of a balance model depends on the variables of interest, the network size, and how it is compartmentalized. Thus, it is easy to imagine how complex a statistical ENA model can be. As a start, we will focus on very simple balance models to demonstrate the rationale and application of our approach. When practical situations call for more complex models, the same principles from this article may be applied to augment the current methodology.

The rest of this article is structured as follows. Section 2 presents the rationale and practical implications of our statistical approach towards mass balance. Technical aspects of our approach involving Bayesian melding are discussed in Section 3. We apply our method to an existing dataset, and the results are discussed in Section 4. Section 5 describes other aspects of interest as possible extensions of our methodology. Conclusions for the article appear in Section 6.
Mass balance is traditionally viewed as a deterministic physical rule that governs the relationship among quantities associated with the volume or mass of any transferable medium such as a chemical substance or energy. Basic concepts about mass balance in ecology can be found in, e.g. Suter (2007).

Let us consider an ecosystem with \( n \) compartments (disjoint), each comprising one or more species. Then, for a given medium, a simple balance model (taken from Ulanowicz, 2004) is

\[
X_i + \sum_{j \neq i} T_{ji} = \sum_{j \neq i} T_{ij} + Y_i + R_i, \quad i = 1, \ldots, n \tag{1}
\]

where the subscripts \( i \) and \( j \) are compartment labels, \( T_{ji} \) is the rate of transfer from \( j \) to \( i \), \( X_i \) and \( Y_i \) are respectively the rate of exogenous transfer to and from \( i \), and \( R_i \) is the rate of dissipation from \( i \). Note that exogenous quantities originate from or terminate outside of the system, while dissipation is lost or wasted to all systems. All rates in (1) are non-negative, and the equation follows the Law of Conservation, or simply, “what comes in equals what goes out.” However, exact balance is not typically observed in practice. Indeed, many rates are not directly observable from the field. Instead, they are often deduced from field data of measurable auxiliary quantities (e.g. different ratios relative to biomass and consumption), taken possibly from various sources. Since this is typically done for any number of transfer quantities over any number of values of \( i \), the summations on either side of an equation such as (1) serve as restrictive constraints that typically render imbalance. In such cases, computer programs such as EwE and EcoNetwrk can be used to adjust observed quantities and/or fill in unobserved quantities subject to “maximum balance.” Observed quantities including auxiliary data are the software input, and the balanced quantities, the output. Ulanowicz (2004) notes that ideally, actual observed values should not be adjusted.

Statistically speaking, the notion of balance imposed on data appears unnatural. Data, directly observed or deduced from the observed, are inherently variable. Modeling the variability is a common statistical exercise used to enhance the understanding of any system from which the data arise. In this regard, mass balance may be imposed perhaps on the expectation of variables instead of the variables themselves. Or simply, “what comes in equals what goes out, on average.” To demonstrate this notion, we consider a much simplified system by combining some terms in (1), as follows:

\[
W_i \equiv X_i + \sum_j T_{ji} = \text{rate of total transfer into } i,
\]

\[
U_i \equiv \sum_j T_{ij} + Y_i = \text{rate of total transfer out of } i \text{ into other compartments or systems},
\]

\[
(\theta_1, \theta_2, \phi) \equiv E(W_i, U_i, R_i) \quad \text{for all } i. \tag{2}
\]
Thus, the statistical notion of mass balance appears as a single equation, namely,

\[ \phi = \theta_1 - \theta_2. \] (3)

The goal is to make inference on each parameter in (3).

Without the constraint of average balance, the sample mean may be a simple but statistically sound estimate of the variable’s expectation. However, (3) now creates a dilemma. Suppose we first estimate \( \phi \). Due to randomness, the sample means \( \bar{R} \) and \( \bar{W} - \bar{U} \) will virtually never coincide. Thus, \( \bar{R} \) is not an ideal estimate of \( \phi \), as it entirely ignores the data \( W_i \)’s and \( U_i \)’s; and vice versa. In rare situations, pooling \( \{W_i - U_i\} \) with \( \{R_i\} \) may suffice, although a different degree of reliability between the two sets of observations otherwise poses an issue for the pooling strategy. Here, distinction must be made between the notions of reliability and variability: the latter is generally attributable to the measuring mechanism, while the former pertains to how honestly the data reflect reality. Specifically, many ENA variables are not directly observable in practice. For the remainder of the article, we will suppose that \( R_i \) is the only variable on the right-hand-side of (2) that is possibly unobservable (since dissipation can be untraceable). Replacing it is \( R_i^* \), a deduced quantity from other means, that is necessarily less dependable than \( W_i - U_i \) that have been directly observed. Even if we additionally assume \( E(R_i^*) = \phi \), the same dilemma remains. A technique to sensibly integrate, or meld, the two sets of information about \( \phi \) becomes necessary. Of course, the relation imposed by (3) implies that the melded inference for \( \phi \) now influences the perception of \( \theta = (\theta_1, \theta_2) \) beyond the basic inference that stems from the sample mean and the Central Limit Theorem (CLT), a common approach had \( \theta \) been estimated independently of (3). The required technique to handle the melding and its influence on \( \theta \) is discussed in Section 3.

2.1 Implications

What, then, are the practical implications once proper inference for \( \phi \) and \( \theta \) is available? First, formal confidence statements that incorporate the notion of balance can be made about mean rates of transfer, which existing ENA techniques cannot provide. In turn, the melded inference for \( \phi \) can be used in an augmented analysis to make confidence statements, accounting for balance, about each individual \( R_i \) that was not observed in the first place (see Section 5).

Second, this type of confidence assessment can be regarded as a “reality check” so that little confidence implies poor data quality or even inappropriate physical theory (recall (a) among Dame and Christian’s criticisms). In either case, any further conclusions drawn for the ecological network would sacrifice scientific integrity. This second feature of our approach is fundamentally different from standard practice of balance modeling in ENA, which coerces balance on data without a formal assessment of data quality / physical theory, then proceeds to draw further conclusions based on the adjusted data.
3  BAYESIAN MELDING FOR MASS BALANCE

Poole and Raftery (2000) developed Bayesian melding as a method of proper statistical inference for deterministic dynamics models in which quantities evolve over time. Their work was embraced by the International Whaling Commission who had traditionally favored non-stochastic population dynamics models derived from differential equations. Like any Bayesian inference techniques, Bayesian melding requires the likelihood for data and the prior distribution of parameters to be prespecified. The key extra component is a prior \( p^*_2 \) for the output quantity that is induced by applying the physical-theoretic model, \( M \), to draws from the prior \( p_1 \) stated for the input quantity. (In general, model output is the set of quantities on which statistical inference is focused. Input quantities are the rest that define the output according to \( M \).) A series of steps follows: (i) the prespecified or premodel output prior \( p_2 \) (stated independently of \( M \)) and induced prior \( p^*_2 \) are melded to form the melded output prior, \( \tilde{p}_2 \); (ii) this \( \tilde{p}_2 \) is fed through \( M^{-1} \) to obtain the melded input prior, \( \tilde{p}_1 \); (iii) then \( \tilde{p}_1 \) is combined with the input and output likelihoods to form the (melded) input posterior distribution, \( \tilde{\pi}_1 \); (iv) finally, \( \tilde{\pi}_1 \) is fed through \( M \) to yield the (melded) output posterior, \( \tilde{\pi}_2 \). Bayesian inference is drawn based on these posteriors.

Now, we demonstrate that Bayesian melding can also be used for the static system (3).

First, we decide on which parameters from (3) are model input and output. (These are not to be confused with material input to and output from a compartment in an ecosystem.) Recall from Section 2 the terms “input” and “output” for mass balance computer programs in the presence of deduced data. Since we assume that \( R_i \)'s are possibly replaced by deduced quantities, they should be subject to the most adjustment if fed into the balance program, leading to a set of program output that likely differs from the input. To parallel this idea, here we may take \( \phi \) to be the physical-theoretic model output in the Bayesian melding context. Then, \( \theta \) is the model input. Hence, the balance model for our statistical ENA is

\[
M : \theta \mapsto \theta_1 - \theta_2 , \quad \phi \equiv M(\theta) .
\]  

Next, we consider (3) for summer carbon transfer in the Chesapeake Bay mesohaline network (Baird and Ulanowicz, 1989), with \( n=36 \) compartments, and transfer rates ranging from 0 to the order of \( 10^6 \) mg/m²/summer. For a more manageable range in computations, we analyze the data in g/m²/summer instead.

We are now ready to proceed with all the steps in Bayesian melding.

3.1  Premodel priors and likelihoods

For the very simple model (3), it is reasonable to assume that expert opinions are available for the premodel joint distribution of \( \varphi \equiv (\theta_1, \theta_2, \phi) \). For the purpose of illustrating our approach, we
replace expert opinions with our somewhat vague intuition based on the types of data shown in Baird and Ulanowicz (1989). In general, expert opinions may not be available for some quantities, especially in more complex models such as the expectation of (1). In such cases, we suggest the use of diffuse priors. The goal is then to specify a reasonable prior that reflects the data type instead of particular datasets. Thus, we note the non-negative transfer rates that tend to be highly right-skewed (Figure 1), and the small $n=36$ that may not drastically reduce the skewness of the mean rate. Then, a trivariate log-normal prior seems reasonable:

$$\log(\varphi) \sim N_3(\mu, \Sigma),$$

with the choice of $\mu$ and $\Sigma$ based on the following rationale. First, according to $M$, it may be reasonable to take $E(\theta_2) = E(\phi) = E(\theta_1)/2$ and $\text{Var}(\theta_2) = \text{Var}(\phi) = \text{Var}(\theta_1)/2$. Next, total incoming rates are typically $w_i = O(100)$ g/m$^2$/sum. That is,

$$100 \approx W_i \approx E(W_i) = \theta_1 \approx E(\theta_1) = \exp\{\mu_1 + \sigma_1^2/2\}. \quad (5)$$

We further note that the sample standard deviation of $w_i$'s is also $O(100)$, but we take $\text{Var}(\theta_1) \approx 100^2/2 = 50000$, as the mean of $W_i$ should be less variable than $W_i$ itself. Hence,

$$50000 \approx \text{Var}(\theta_1) = (\exp\{\sigma_1^2\} - 1) \exp\{2\mu_1 + \sigma_1^2\}. \quad (6)$$

Solving (5) and (6) for $\mu_1$ and $\sigma_1^2$ yields $\mu$ and the diagonal entries of $\Sigma$. For off-diagonals, we consider an exchangeable correlation structure, with a pairwise correlation of 0.5. Positive correlations reflect the notion that $W_i$, $U_i$, and $R_i$ tend to increase and decrease together as a triplet (this is analogous to the income, spending, and savings of a randomly selected person). The choice of 0.5 reflects our ignorance about the extent of the dependence.

With their inherent skewness, transfer rates are modeled to have exponential likelihoods:

$$W_i|\theta_1 \iid \exp(1/\theta_1), \quad U_i|\theta_2 \iid \exp(1/\theta_2), \quad R_i|\phi \iid \exp(1/\phi),$$

$$W_i, U_i, R_i|\phi \text{ mutually independent.} \quad (7)$$

Of course, the notion of balance imposes dependence among $W_i$, $U_i$ and $R_i$. This is reflected by their marginal joint distribution through $\Sigma$.

### 3.2 Induced output prior and melded input prior

Marginalize the trivariate log-normal premodel prior according to the input and output components, and denote them by $p_1(\theta)$ and $p_2(\phi)$, respectively. Now, $M$ takes the draws from $p_1$ to the $\phi$-space, leading to an induced output prior, denoted by $p_2^*(M(\theta))$. 

Next, the melding of $p_2^*$ with $p_2$ to form $\tilde{p}_2$ is considered. However, it is a mere intermediate step that precedes the computation of the melded input prior $\tilde{p}_1$. Poole and Raftery (2000) prove that logarithmic pooling of $p_2^*$ and $p_2$, taken back to the $\theta$-space, yields the melded input prior

$$\tilde{p}_1(\theta) \propto p_1(\theta) \left[ \frac{p_2(M(\theta))}{p_2^*(M(\theta))} \right]^{1-\alpha}, \quad \alpha \in [0, 1]. \quad (8)$$

Conveniently, (8) eliminates the explicit evaluation of $\tilde{p}_2$, yet maintains the proper notion of inversely mapping $\tilde{p}_2$ even if $M^{-1}$ does not exist due to a smaller dimension for $\phi$ than $\theta$.

Note that (8) is but the premodel input prior, $p_1$, weighted by the premodel and induced output priors; the pooling weight is $\alpha$. Poole and Raftery (2000) argue that the choice of $\alpha$ should depend on the reliability of prior information provided through $p_1$ (that induces $p_2^*$ and $p_2$). In the context of ENA, we suggest that $\alpha$ should additionally reflect the relative dependability of the input data to the output data, the latter of which are often deduced, i.e. less dependable. For the purpose of illustration in this article, we take $\alpha=0.5$.

### 3.3 Melded input and output posteriors

The final step in Bayesian melding is to obtain the input and output posteriors for proper Bayesian inference. First, for the input,

$$\tilde{\pi}_1(\theta|W, U, R) \propto p(W, U, R|\theta) \tilde{p}_1(\theta) \nonumber$$

$$= \prod_{i=1}^{n} p(W_i|\theta_1) \ p(U_i|\theta_2) \ p(R_i|M(\theta)) \ \tilde{p}_1(\theta). \quad (9)$$

Apply $M$ again to map the draws from (9) to the $\phi$-space, thus yielding the melded output posterior $\tilde{\pi}_2(\theta|W, U, R)$.

### 4 APPLICATION TO THE CHESAPEAKE BAY MESOHALINE NETWORK

Data from Baird and Ulanowicz (1989) are broken into the four seasons of the year, and presented in the form of network flow “spaghetti” diagrams. Instead of extracting data from these, we located the summer data online (http://www.cbl.umces.edu/~ulan/ntwk/datall.zip). Discrepancy exists between the spaghetti diagrams and online data; we attribute it to the latter having already been balanced. Nevertheless, we proceed with these data to illustrate our statistical ENA inference methodology, and continue to regard $\phi$ as the model output. In practice, we suggest that melding be applied to pre-balanced data, so that the statistical inference can serve as an assessment of the appropriateness of the data at hand for mass balance theory.
All steps in Section 3 involve evaluating density functions. Note that closed forms are only available for the premodel priors and likelihoods. To evaluate the other densities, we employ numerical algorithms for kernel density estimation, linear interpolation (for evaluating all kernel density estimates over the same set of support points to estimate $\tilde{p}_1$ in (8)), and sampling from (9). The latter is implemented using an algorithm for Metropolis-Hastings within Gibbs sampling, a Markov chain Monte Carlo (MCMC) technique. Implementation details for all steps from Section 3 are available in Gould (2008).

4.1 Results

Our Bayesian inference for $\varphi$ is based on two independent sets of 4 000 post-burn-in MCMC samples from the melded posteriors. The trace plot in Figure 2 shows substantial overlap between chains (shown in black and gray), indicating good mixing. Their levelness also indicates convergence to the target distributions. Thus, we combine both chains and examine them as a single sample. Some posterior summary statistics appear in Table 1. Note the high agreement between means and medians, and between the lower / upper quartiles and the 95% highest posterior density (HPD) intervals. This reflects the approximate symmetry of the posteriors, as is evident in the histograms shown in Figure 3. The figure also shows a drastic difference between the posteriors and premodel priors, suggesting that the latter contribute little to the Bayesian inference. The same can be said about the melded priors, which are again extremely skewed (not shown here; see Gould, 2008).

Results from our approach may be compared to the standard classical counterpart based on the CLT. Although the point estimate for $\varphi$ is expectedly almost identical between the two approaches, the precision is drastically different between the two estimates. This is evident in the CLT-based interval estimates that are about three times as wide as the Bayesian HPD intervals (Table 1).

Another point to be highlighted is the correlation structure among the three mean transfer rates. Figure 4 breaks down the joint melded posterior of $\varphi$ into bivariate components. It is evident that the two mean transfer rates are very highly correlated ($\rho \approx 0.9$), although the mean dissipation rate is much less correlated with either mean transfer rate ($\rho < 0.4$ with $\theta_1$ and $\approx -0.1$ with $\theta_2$). This dependence structure presents itself as possibly new insight for the ecologist: the (re)cycling of media (e.g. matter and energy) within a closed system necessarily imposes interdependence among transfer rates. However, our inference reveals a much weaker interdependence when transfer rates are averaged over all compartments in the ecosystem.

Note that insight into the correlation structure among mean transfer rates is a convenient consequence of Bayesian inference through the joint posterior, regardless of melding. In contrast, standard classical inference regards population means as constants, thus limiting the inference to the estimation of the constants without yielding further wisdom.
5  POSSIBLE EXTENSIONS

When a transfer rate cannot be directly measured, prediction inference for it may be desirable. Thus far, we have assumed that both the unmeasurable and its proxy (deduced from other sources) share the same mean. Then, with the proxy data, Bayesian melding as described above provides proper inference for this mean. If one is to further model the relationship between the unobserved and deduced, perhaps through a simple regression model, then the unobserved can be treated as missing data, for which Bayesian imputation via posterior predictive methods is straightforward. Specifically, the statistical ENA now can be augmented by including the unobserved variable alongside others that already appear in the original ENA, as well as the modeled relationship between it and its proxy. The proxy then serves as auxiliary information for the unobserved to help in its prediction, while also making contribution to the inference for the shared mean.

Another direction of extension is to consider multiple transfer media simultaneously. Ulanowicz (2004) points out that conventionally, each medium of interest defines a separate network, even if the same ecosystem of compartments is repeatedly studied but over different media. When multiple media are of simultaneous interest, special techniques (mostly based on information theory) are then used for analyzing networks in parallel. On the other hand, it may appear that such an issue can be easily handled statistically by incorporating a block index $k$ to (3), then repeating the exercise of Bayesian melding as above. Specifically, the statistical component of the model would require priors to be stated for each medium, and, if necessary, also for the interdependence of parameters over the $k$ equations. Melding for the latter may not be needed, as conventional mass balance models do not dictate the connectance among media. For each type of transfer (e.g. dissipation), one can treat the $k$ parameters as a vector, and proper multivariate or marginal inference can then be drawn for inter-compartmental transfer of the given type over different media.

6  CONCLUSION

This article has featured a new statistical approach towards ENA, integrating statistical modeling of data with physical-theoretic modeling of underlying quantities. The latter is favored by the ecological community over purely empirical approaches such as regression techniques which form the basis of standard statistical methodologies. The physical model used to demonstrate our approach is likely the least complex in practical situations; therefore, this article may be regarded as a primer on the rationale and principles of employing Bayesian melding for studying ecological networks. Future articles to appear will extend the current principles to analyze more complex ecological networks. The extension is straightforward, although it can be computationally intensive.

Despite the use of a least complex balance model in this article, we have demonstrated that
Bayesian melding as a statistical inferential technique for ENA is practical and scientifically sound. It allows a direct assessment of the appropriateness of data for mass balance modeling, and preserves a level of “honesty” by acknowledging the natural conflict between randomness and physical theory. The extra level of uncertainty due to the use of indirectly observed data can also be properly incorporated into the analysis with little ambiguity. Finally, as a desirable side-effect of its being Bayesian, the inference can provide new ecological insight about the interdependence of model parameters that would be lacking from standard frequentist inference.

Note that due to the existing balance in our data here, the classical approach for estimating $\phi$ could not have utilized the pooling of $\{W_i - U_i\}$ with $\{R_i\}$. Even if it could have for pre-balanced data, the reliability concern as discussed in earlier sections leads to ambiguity in the pooling scheme. In contrast, this issue can be properly handled by Bayesian melding, as long as the relative reliability between directly observed and deduced datasets can be sensibly expressed through the logarithmic pooling weight, $\alpha$.

To keep the focus of the current article, components appearing as “possible extensions” have yet to be demonstrated. It is our intention to provide details of these extensions in future articles.

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REFERENCES


Chiu GS, Westveld AH. In progress. Statistical inference for food webs via longitudinal social network models.


Table 1: Bayesian inferential statistics based on melded posteriors, with classical summaries provided for comparison; HPD and CLT intervals correspond to 95% confidence

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$\theta_1$</th>
<th>$\theta_2$</th>
<th>$\phi$</th>
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<td></td>
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<tr>
<td>CLT interval</td>
<td>(33.24, 146.06)</td>
<td>(20.70, 110.56)</td>
<td>(4.24, 43.80)</td>
</tr>
</tbody>
</table>
FIGURES

Figure 1: Histograms of carbon flow (g/m^2/summer) for the Chesapeake Bay mesohaline network (online data)

Figure 2: Trace plot for two overlaid chains of MCMC samples (after burn-in) from the melded posteriors (Chain 1 in black, and Chain 2 in gray; from top to bottom: θ_1, θ_2, and φ)
Figure 3: Histograms of melded posterior samples (black), overlaid with premodel prior densities (gray)

Figure 4: Pairwise joint melded posteriors based on MCMC samples (density values increase from white to black)