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Abstract: Objectively assessing the performance of a model and deriving model parameter values from observations are critical challenges in ecosystem modeling. In this paper, we applied a nonlinear inversion technique to calibrate the ecosystem model CENTURY against carbon (C) and nitrogen (N) stock measurements collected from 33 mature tropical forest sites in five life zones in Costa Rica. Net primary productivity (NPP) from the Moderate Resolution Imaging Spectroradiometer (MODIS), C, and N stocks in aboveground live biomass, litter, coarse woody debris (CWD), and soils were used to calibrate the model. To investigate the resolution of available observations on the number of adjustable parameters, inversion was performed using nine setups of adjustable parameters. Statistics including observation sensitivity, parameter correlation coefficient, parameter sensitivity, and parameter confidence limits were used to evaluate the information content of observations, resolution of model parameters, and overall model performance. Results indicated that soil organic carbon content, soil nitrogen content, and total aboveground biomass carbon had the highest information contents, while measurements of carbon in litter and nitrogen in CWD contributed little to the parameter estimation processes. The available information could resolve the values of two to four parameters. Adjusting just one parameter resulted in underfitting and unacceptable model performance, while adjusting five parameters simultaneously led to overfitting.

1. INTRODUCTION

Numerical models are frequently used to characterize and predict landscape processes and consequences. Most landscape modeling efforts rely on deploying classic plot-scale models in space using various spatial databases as input data and driving forces (Reiners et al., 2002; Liu et al., 2004a, 2004b). One of the main challenges of this approach is the difficulty in quantifying the spatial variability of model parameters. Conventionally, one or multiple lookup tables are often used to

prescribe the variability of some sensitive parameters across various strata (usually by land cover, plant functional type, or biome) in the study area. In this case, each stratum will have a unique combination of parameter values. Although this approach deals with parameter variability to a certain degree, it ignores the impact of additional environmental factors on parameter variability. Because of the variability of parameter values, model calibration is often needed to find the optimal set of parameter values for any given site (Wang et. al., 2001). For modeling processes over large areas,

it is ideal that spatially explicit parameter surfaces or fields can be generated or available. Otherwise, the simulated spatial patterns might be flawed or even incorrect.

Nonlinear inversion has been used in other research, yet this study is the first time this technique has been applied to Carbon and Nitrogen dynamics. To overcome the shortcomings of conventional calibration, we applied a nonlinear inversion technique to calibrate the ecosystem model CENTURY against carbon stock measurements collected from 33 mature tropical forest sites in five life zones (tropical dry, tropical moist, tropical wet, tropical premontane rain, and tropical premontane wet) in Costa Rica (Fig. 1).

2. METHODS

2.1 Observations

Diameters at breast height of live and dead trees were measured for all of the trees in the field plots. Carbon (C) stocks in aboveground live biomass and coarse woody debris were then estimated using allometric equations that relate diameter at breast height (DBH) of a tree to its C content.

Carbon stocks on the forest floor and in soil were also measured. C and nitrogen (N) ratios of aboveground biomass, coarse woody debris, litter, and soils were measured and used to estimate N stocks in these compartments. Soil bulk density and texture were also measured at these sites.

Annual net primary productivity (NPP) of these sites was derived from MODIS. To minimize errors, the maximum annual NPP within a 5-km-by-5-km window was extracted from the MODIS NPP surface in 2001. This maximum NPP was assumed to represent the annual NPP of the mature forest site and used in model calibration as well.

Surfaces of average monthly precipitation

Figure 1. Sites for measuring C and N stocks.

and monthly maximum and minimum temperatures, which are required to run the CENTURY model, were generated by Kriging data collected from weather stations. Climate data for each of the field sites were then extracted from the surfaces according to their geographic locations.

2.2 CENTURY Model

The CENTURY model was designed to simulate C, N, phosphorus, and sulfur cycles in various ecosystems including crops, pastures, forests, and savannas worldwide (Parton et. al., 1987). The model inputs included climate data, soil data, biological data, management practices, and disturbances. At the end of each model run (when C and N stocks in the system become relatively stable), simulated C and N values were compared with the field measurements. If the difference was large, another set of model parameters was used and the model was run again. This searching for optimal parameter values used a nonlinear inversion technique implemented in the Model-Independent Parameter Estimation (PEST) software package (PEST, 2003).

2.3 Nonlinear Inversion

2.3.1 PEST

The goal of nonlinear inversion is to derive a set of model parameter values that minimize the least squares of the weighted residuals. PEST adjusts model parameters until the fit between model outputs and field observations is optimized. PEST takes control of the model, running it as many times as necessary to determine the optimal set of parameters. In PEST, determining the optimal set of parameters is achieved by calculating the mismatch between the model output and the observation data, determining the best way to correct the mismatch, adjusting the values of the model parameter values, running the model again, and repeating the process until the results are close to the observation data.

2.3.2 Diagnostic and Inferential Statistics for Inverse Modeling

The statistics used by PEST for determining optimal parameter values include parameter sensitivity, observation sensitivity, parameter correlation coefficients, and overall model fit. Parameter

sensitivity indicates how easily parameters can be estimated by regression. Parameters with high sensitivity values are easier to estimate than those with low values. Observation sensitivity is a measure of the sensitivity of the observation to all parameters in the estimation process. Higher observation sensitivity implies more information from observations has contributed to the estimation process. Parameter correlation coefficients suggest the likelihood that estimated parameter values are likely to be unique. High correlation coefficients are indicative of a high degree of uncertainty in the parameter estimation process and also indicate non-uniqueness. Overall model fit was determined through two methods. The first was a visual inspection of the pattern of residuals. A small residual close to zero indicates a good model fit. The second method for model fit was a linear regression between observed and simulated values. A successful model fit satisfied the following conditions: (1) the linear regression is significant at $\alpha = 0.01$, (2) the slope of the regression is not significantly different from 1 at $\alpha = 0.005$, and (3) the intercept of the regression is not significantly different from 0 at $\alpha = 0.005$.

2. 4 Modeling and Experiment Design

Each of the nine PEST/CENTURY model runs consisted of each of the 33 mature forest sites being optimized individually by the model with each of the runs having a different set of adjustable, tied, or fixed parameters (Table. 2).

All the sites within each run used the same combination of adjustable parameters. By changing their combinations of adjustable parameters and their weights, the results could be compared to see how relationships changed and how a particular parameter might affect the optimization process. The combinations of parameters used in each are not always unique because the weights of some parameters were changed. Weights were assigned to each of the observations to reflect the magnitude of the values and the quality of the data. The weights for the observations changed in different runs to investigate the importance of the observation data on model inversion. Parameters that were adjustable or tied were significant because they were optimized based on the model and observation data.

3. RESULTS

3.1 Observation Sensitivity

Three conclusions can be made about observation sensitivities from this study. First, sensitivities of a given observation for a given model run varied from 1 to 5 magnitudes across all sites. This indicates that the amount of information contained in an observation varied from site to site. Second, the sensitivities of different observations varied greatly, and the medians differed by several magnitudes. Third, observation sensitivities varied among model runs due to different combinations of adjustable parameters or weights being used for each run.

3.2 Parameter Sensitivity

For the 33 sites in this study, parameter sensitivities were lower in the tropical dry and moist life zones, likely indicating that field data collected in these two life zones contained less information about these parameters. The variability of parameter sensitivities among sites suggests that the available data resolved optimized parameters differently.

Table 2. Adjustable (V), tied (T), and fixed (F) parameters for the nine model runs. Letters after T represent the parameter to which the indicated parameter is tied.

Parameter	ID	1	2	3	4	5	6	7	8	9	Parameter Definition
					Model Run						
dec11	(a)	V	V	V	V	F	T(b)	T(d)	T(d)	F	maximum surface structural decomposition rate
dec4	(b)	V	V	V	V	F	V	T(d)	T(d)	F	maximum decomposition rate of soil organic matter with active turnover
dec5	(c)	T(b)	T(b)	T(b)	T(b)	F	T(b)	T(d)	T(d)	F	maximum decomposition rate of soil organic matter with slow turnover
prdx4	(d)	V	V	V	V	V	V	V	V	V	maximum gross forest production
decw1	(e)	V	V	V	F	F	F	F	F	F	maximum decomposition rate constant for dead fine branches
decw2	(f)	T(e)	T(e)	T(e)	F	F	F	F	F	F	maximum decomposition rate constant for large wood
wooddr2	(g)	V	V	F	F	F	F	F	F	F	monthly death rate fraction for fine roots
wooddr3	(h)	T(g)	T(g)	F	F	F	F	F	F	F	monthly death rate fraction for fine branches
wooddr4	(i)	T(g)	T(g)	F	F	F	F	F	F	F	monthly death rate fraction for large wood
wooddr5	(j)	T(g)	T(g)	F	F	F	F	F	F	F	monthly death rate fraction for coarse roots
teff2	(k)	---	---	---	---	--	---	---	---	V	minimum temperature for vegetation growth

3.3 Parameter and Correlation Coefficients

Figure 3 shows the correlation coefficients between adjustable parameters for model run 1. Runs 5, 7, and 8 had only one adjustable parameter, so they did not have a correlation coefficient. Correlation coefficients for the same parameters varied from site to site and from run to run. There was no single pair of parameters that were consistently correlated. Correlation coefficient outliers might indicate that the model was difficult to optimize when applied to some sites.
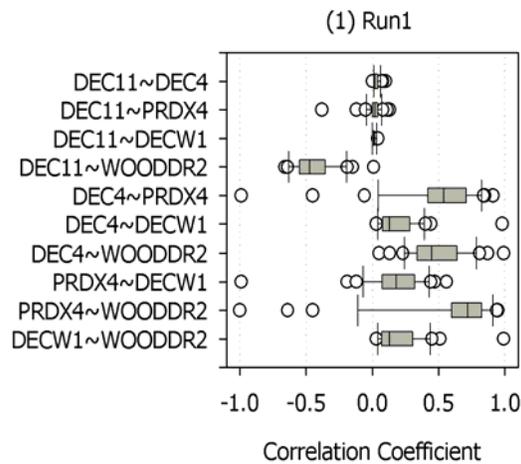

Figure 3. Run 1 correlation coefficients.

According to Poeter and Hill (1998), a correlation coefficient larger than 0.90 suggests that the parameters are correlated, and hence, the values of parameters would be highly uncertain. No single pair of parameters was consistently correlated (i.e., none had correlation coefficient > 0.90 all the time).

3.4 Parameter Uncertainty

Figure 4 shows the optimized parameter values and their corresponding 95% confidence intervals. Results suggest that the confidence intervals of DEC11 (Figs. 4 A1–A2) and DECW1 (Figs. 4 F1–F2) were consistently wider than other parameters across all of the model runs and all of the sites. The confidence intervals of PRDX4 varied among model runs (Figs. 4 D1–D2) with the smallest intervals for runs with 2 to 4
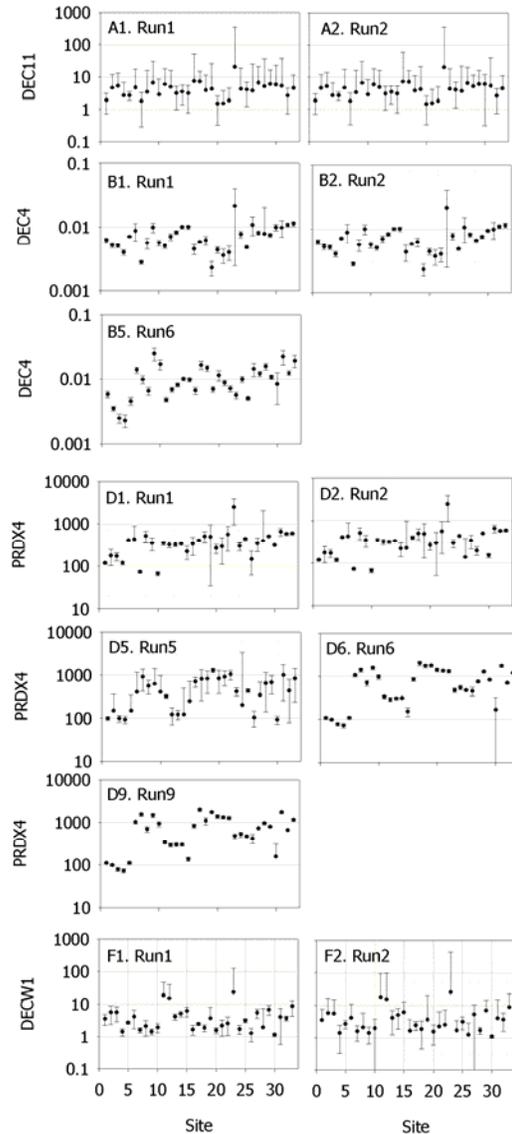

Figure 4. Selected confidence intervals.

optimized parameters, intermediate intervals for runs with 5 optimized parameters, and wider intervals for runs with only 1 optimized parameters.

The large confidence intervals of DEC11 and DECW1 agreed with the observations from parameter sensitivities that these two parameters were relatively insensitive because limited information was contained in the observations about these two parameters. This suggests that both over- and under-fitting are likely to increase the uncertainty of parameter values for a given set of observations. All other parameters were well resolved as suggested by their small confidence intervals. In general, DEC4 was better resolved than any other parameters.

3.5 Goodness of Model Fit Across Sites

Figure 5 shows a comparison between simulated and observed values for all nine model runs across the 33 sites with the following results: (1) 50 of 81 comparisons showed that simulated values were significantly different from observations, (2) simulated LITTERN and WOODN values were significantly lower than observations, which was consistent across all model runs, (3) all simulations were significantly different from their corresponding observations for all of the variables in run 7 and run 8, and (4) no relationship existed between simulated and MODIS NPP values, except runs 1 and 2, and the number of matches between simulated and observed values increased with increasing numbers of adjustable parameters.

4. DISCUSSION

The agreement between simulated and observed values increased with an increasing number of adjustable parameters n. This is consistent with the general trend that a perfect fit can always be reached by increasing n as a result of overfitting. In this study, the maximum n used was 5, resulting in the highest agreement between simulated and observed values. We believe that n with a value of 5 has already resulted in overfitting some observations, notably MODIS NPP (Fig. 5). The overfitting of NPP in Run1 and Run2 does not mean all of the observations have been overfitted. In fact, LITTERN and WOODN are still poorly fitted.

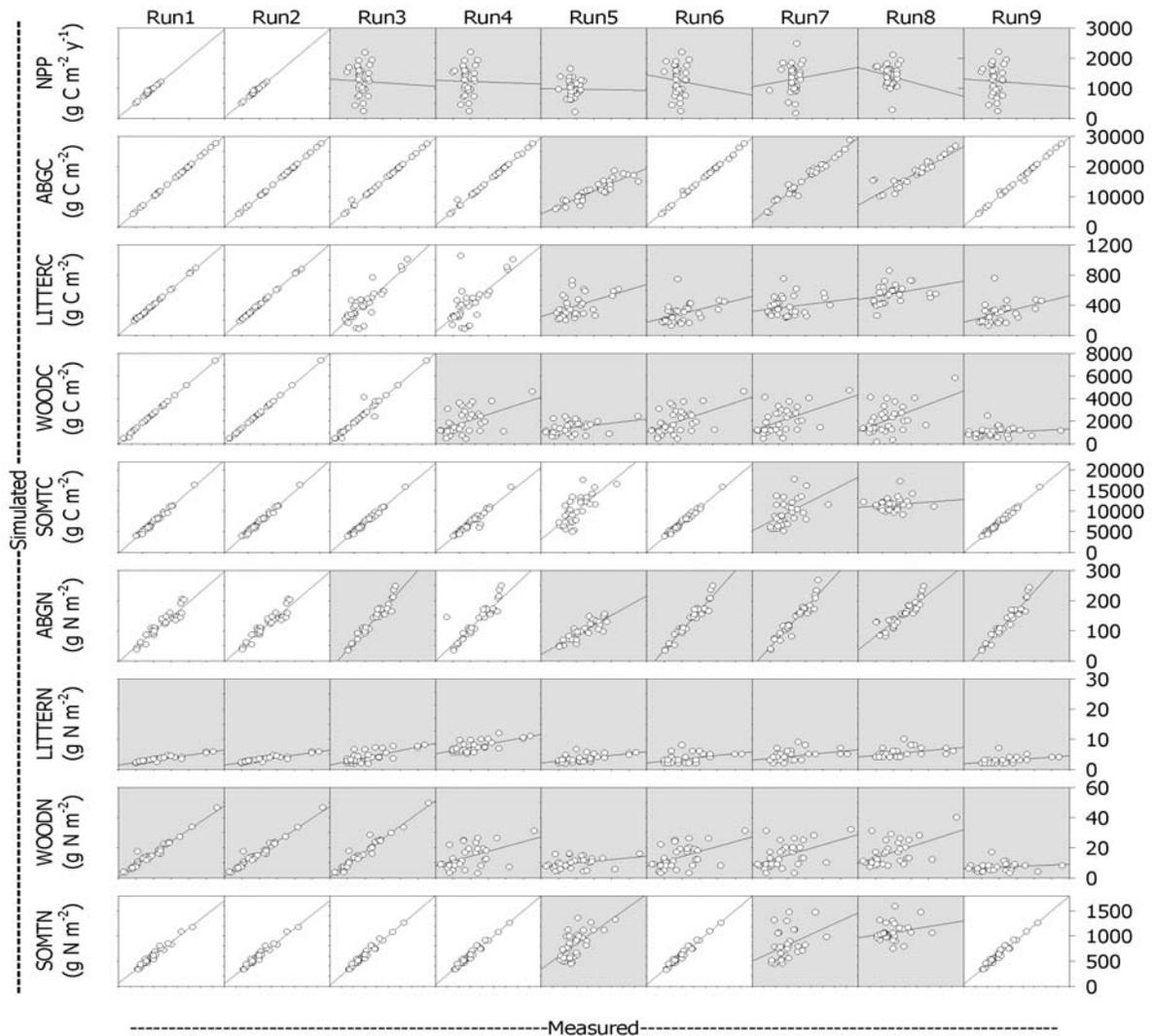Underfitting may happen if the number of adjustable parameters is not enough, as demonstrated

Figure 5. Goodness of Model Fit.

by Run5, Run7, and Run8. These runs suggest that adjusting PRDX4 and its tied parameters was not enough to take advantage of the information contained in the observations. The failure of tying decomposition coefficients to PRDX4 to explain the variances in observations also suggested that the spatial variations of DEC11, DEC4, and DEC5 were not well coupled with production.

Our results showed that the values of 2 to 4 parameters can be successfully resolved with the available information. Underfitting can result from only one adjustable parameter, leading to a failure of comparison between simulated and observed values. Adjusting more than four variables could result in overfitting at least partially.

This study demonstrates that some model parameter values can be resolved, and the key carbon flux, NPP, at the ecosystem level can be inferred from C and N stock measurements using nonlinear model inversion. To our knowledge, C and N stock measurements have not been used in this context before. The results of this study have several important implications. First, this method might be used to derive model parameter and NPP values from C stock measurements in mature forests. Such measurements may have already been acquired by national to regional forest inventory systems in various places in the world. Second, because of the difficulties involved in the estimation of NPP using observational approaches (Clark et al., 2001) and their importance in the carbon cycle, the ability to infer NPP values from C stock measurements in mature forests can contribute significantly to our understanding of the global to regional carbon cycle. The NPP databases generated using this approach can be used to improve the calibration and validation of NPP algorithms, and therefore, potentially enhance our capability and accuracy of predicting NPP using remote sensing technologies. Third, the optimized parameter values can be analyzed to develop predictive relationships with site conditions such as precipitation and temperature as well as other parameters. Parameter surfaces can then be generated from these predictive relationships to support the deployment of the model in space.

5. ACKNOWLEDGMENTS

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