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Simulating CO_2 flux of three different ecosystems in ChinaFLUX based on artificial neural networks

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Abstract The nonlinearity of the relationship between CO_2 flux and other micrometeorological variables flux parameters limits the applicability of carbon flux models to accurately estimate the flux dynamics. However, the need for carbon dioxide (CO_2) estimations covering larger areas and the limitations of the point eddy covariance technique to address this requirement necessitates the modeling of CO_2 flux from other micrometeorological variables. Artificial neural networks (ANN) are used because of their power to fit highly nonlinear relations between input and output variables without explaining the nature of the phenomena. This paper applied a multilayer perception ANN technique with error back propagation algorithm to simulate CO_2 flux on three different ecosystems (forest, grassland and cropland) in ChinaFLUX. Energy flux (net radiation, latent heat, sensible heat and soil heat flux) and temperature (air and soil) and soil moisture were used to train the ANN and predict the CO_2 flux. Diurnal half-hourly fluxes data of observations from June to August in 2003 were divided into training, validating and testing. Results of the CO_2 flux simulation show that the technique can successfully predict the observed values with R^2 value between 0.75 and 0.866. It is also found that the soil moisture could not improve the simulative accuracy without water stress. The analysis of the contribution of input variables in ANN shows that the ANN is not a black box model, it can tell us about the controlling parameters of NEE in different ecosystems and micrometeorological environment. The results indicate the ANN is not only a reliable, efficient technique to estimate regional or global CO_2 flux from point measurements and understand the spatiotemporal budget of the CO_2 fluxes, but also can identify the relations between the CO_2 flux and micrometeorological variables.

Keywords: artificial neural network, CO_2, ChinaFLUX, energy flux, variables contribution.

The net ecosystem exchange (NEE) between vegetation and atmosphere is important for understanding carbon sinks and sources. To predict global climate change requires quantifying and observing NEE of different ecosystems on a long-time basis, researching spatial distribution of NEE and simulating dynamic change of NEE.

In recent years, the eddy covariance technique is not only applied to measuring ecosystem CO_2 exchange across a spectrum of time scales, ranging from hours to years, but also used to measure spatial distribution of NEE with a footprint ranging from a few meters to a kilometer depending on the tower height. The need to understand CO_2 flux at other locations or a larger region requires observations as a large number of point or modeling approach. Resources and practical limitations to monitor large areas justify a modeling approach to understand spatial distribution of carbon flux between the atmosphere and a plant canopy[1]. Research result shows that CO_2 flux is correlated to the energy fluxes (latent heat and sensible heat) and environmental variables such as temperature (air, soil and surface), soil moisture and others, which makes it easier to apply statistical learning techniques based on machine learning for CO_2 simulation. The artificial neural networks (ANN) are among the techniques based on pattern recognition capable of modeling non-linear processes. The application of ANN techniques to ecosystem carbon estimation is one of the new areas of data-driven modeling utilizing the relationship among the micrometeorological variables. Recently, researchers applied the ANN techniques for simulating ecosystem carbon flux[2−9]. Van Wijk *et al.*[6,9] used ANN in the top-down approach to model CO_2 and water fluxes from six different coniferous forests in Europe. The study used global radiation, temperature, vapor pressure deficit as input variables to predict CO_2 flux. The results indicated that independent predictions of forest ecosystem fluxes were equally satisfied as empirical models and both water and carbon fluxes can be modeled without detailed physiological and site specific information[6]. Papale *et al.*[7] also used ANN techniques to fill gap of flux tower data and integrate land use, NDVI data to model spatial (1 km×1 km) and temporal (weekly) of carbon fluxes for European forests at continental scale[7]. Development of inverse methods in remote sensing provides the advantage for obtaining the energy flux data at regional scale[10]. The nonlinear relationship between energy fluxes, environmental variables and CO_2 fluxes increases the difficulty for model simulating, but it provides a new method to integrate inverse methods of remote sensing, to model spatial distribution of CO_2 fluxes at regional or continental scale. Assefa *et al.*[8] used energy fluxes and temperature (soil, air) as input variables to model CO_2 fluxes of three different ecosystems in Ameriflux[8]. Although the result is perfect, the research simply shows that the soil moisture will improve the model accuracy, and no further study has been conducted on soil water content and on the ANN technique which explains the process mechanism. All these researches conclude that the ANN approach can be useful for gap filling and carbon flux spatialization[6−9,11].

The overall objective of our study is to evaluate the performance of ANN modeling of CO_2 flux from energy fluxes and temperature (air and soil), and provide the method of simulating the carbon fluxes at regional/continental scale for integrating the remote sensing and flux tower data. Missions include: i) To assess the applicability of ANN-based CO_2 flux simulation for various ecosystems; ii) to study the impact of soil moisture on simulation accuracy; iii) to identify the interactions between micrometeorological variables and carbon fluxes, which have close correlations under different contexts.

1 Methods and data

1.1 Artificial neural networks

An artificial neural network (ANN) is a nonlinear, parallel information processing paradigm that is inspired by the biological nervous systems, such as the brain, process information. It is mainly characterized by high dimension, high degree of interconnection and adaptive interaction between elements. An ANN consists of a set of highly interconnected processing elements (neuron, or units, nodes). Each unit (neuron) accepts a weighted set of inputs and responds with an output. Neural networks have been applied in a wide variety of areas, including speech synthesis, pattern recognition, diagnostic problems, medical illnesses, robotic control and computer vision. In addition, they are able to deal with incomplete information or noisy data and can be very effective to define the rules or steps that lead to the solution of a problem, especially when a mathematical equation is not available[2−4].

Based on connection type and signal transformation direction, neural network types can be classified into feed-forward network and recurrent network. According to different algorithms, the feed-forward network includes Back-Propagation neural network (BPN) and Radius Basic function neural network. In the study, we have used a feed-forward back propagation neural network (BPN).

A standard BPN is composed of input layer, one or more hidden layer and one output layer. Each node is only connected by adjacent node. Nodes at the same layer are not connected with each other. Fig. 1 presents the topological architecture of BPN. ANN (n,m,p,q) is a network including input layer with n inputs, hidden layer with p neurons, output layer with q neurons, m hidden layers with p neurons. When $X_i(i=1,2,\ldots n)$ is input variables, $Y_k(k=1,2,\ldots q)$ is output variables, W_{ij}^h ($i=1,2,\ldots n$, $j=1,2,\ldots p$) is connect weight between input layer and hidden layer, W_{jk}^h ($j=1,2,\ldots p, k=1,2,\ldots q$) is connect weight between hidden layer and output layer, Z_j^h is output values of each hidden layer. The equation is as follows:

$$Z_j^h = f(s_j) = f(\sum w_{ij}^h x_i + \theta_j),$$
$$(i=1,2,...n;\ j=1,2,...p), \tag{1}$$

where $f(s_j)$ is sigmoid function of neuron, also called activation function. s_j is input of j units (neuron), θ_j is critical value. In eq. (1), based on the output layer, $i=1,2,...p; j=1,2,...q$. When network with m hidden layers, $h=1,2,...m$; and when $h>1$, $i=1,2,...p$. $f(s_j)$ usually has $\tan sig_{(s_j)}$ or $\log sig_{(s_j)}$ transfer function, their equation is as follows:

$$\log sig_{(s_j)} = \frac{1}{1+e^{-s_j}} \text{ or } \tan sig_{(s_j)} = \frac{e^{s_j} - e^{-s_j}}{e^{s_j} + e^{-s_j}}. \tag{2}$$

In the study, we have used $\log sig_{(sj)}$ transfer function.

When learning mode of input variables X_i (i = 1, 2, ⋯, n) and architecture of BPN is provided, we may use suitable algorithm to train ANN. During training a network, when error (E) between the outputs $\hat{y}_i$ for the network and actual outputs y_i is less than or equal to a critical value (E_0), also $E \le E_0$, an ANN model is developed with corresponding network architecture and parameters. Error equation is as follows:

$$E = \frac{1}{2}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2. \tag{3}$$

When network architecture and algorithm is selected, modeling dataset is generally divided into three groups: training dataset, used to determine the weights during neural network training; test dataset, used during network training to calculate the errors to prevent overtraining; and validation dataset, used to assess the network's performance with 'new' data, which removes the possibility of the network over fitting on training and test sets. We can apply the trained BPN for modeling the output of new data, also the generalization function of ANN model.

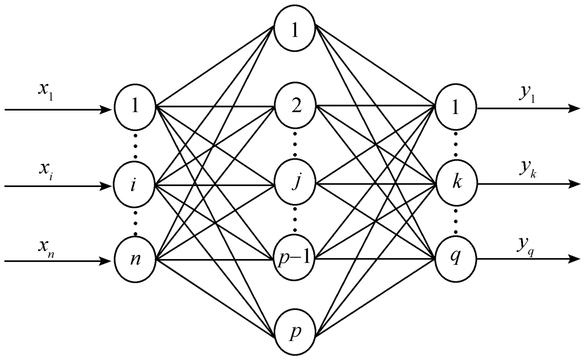

Fig. 1. Topology architecture of BPN.

1.2 Sites descriptions and data

Three different ecosystems (forest, grassland and cropland) at different locations (Changbai Mountains, Haibei, Yucheng) are involved in this study. The sites are part of ChinaFLUX, where CO_2, water vapor, energy fluxes and other biophysical flux and micrometeorological data are measured on a long term and continuous basis[1]. Fluxes and micrometeorological data from these sites are used to train the neural network and predict CO_2 fluxes. The site description, environmental variables monitored and instrumentation for each site are indicated in Table 1. In each ecosystem, we select pre-processed half-hourly data from June to August in 2003 (in Yucheng site, the data start from 15, June), totaling three datasets. Based on each site, we randomly select 60% of dataset as training dataset, 20% as test dataset and 20% as validation dataset.

Table 1 Descriptions of sites

Sites	Changbai Mountains	Haibei	Yucheng
Lon.(°E)	128.0958	101.3000	116.6000
Lat.(°N)	42.4025	37.6000	36.9500
Ecosystem	broad-leaved Korean pine mixed forest	alpine shrub	cropland
Species	*Pinus koriaensis,Tilia amurensis, Quercus mongolica*	*Potentilla fruticosa*	summer maize
Climate	temperate, continental monsoon climate	continental monsoon climate	semi-humid and monsoon climate
MAP (mm)	695	580	520
MAT (°C)	3.6	−1.7	13.1
Soil type	montane dark brown forest soil	Mollic Gryic Cambisols soil	moisture soil, salinized moisture soil
Elevation (m)	738	3200	20
Tower height (m)	40	2.2	2.2
Topography	flat	flat	flat
Beginning data	2002	2002	2002

1.3 Data pre-processing

In order to improve the simulating accuracy, data need to be preprocessed before analysis. In this study, data preprocessing consists of two parts: preprocessing of flux data and normalizing of all data. Preprocessing of flux data includes processing abnormal value and skipping the night-time flux. In processing abnormal value, we refer to FLUXNET whose critical value is indicated in Table 2[12]. Night-time fluxes are skipped from the dataset when wind speed is below 0.12 $m \cdot s^{-1}$ (Yucheng), 0.2 $m \cdot s^{-1}$ (Changbai Mountains), 0.2 $m \cdot s^{-1}$ (Haibei)[13−15].

Table 2 Maximum and minimum values of key variables (FLUXNET, 2003)

Variables	Symbol	Minimum	Maximum
CO_2 flux ($Umol \cdot m^{-2} \cdot s^{-1}$)	*Fc*	−40	40
Friction velocity ($M \cdot s^{-1}$)	*Ustar*	0	6
Latent heat flux ($W \cdot m^{-2}$)	*LE*	−100	700
Sensible heat flux ($W \cdot m^{-2}$)	*H*	−300	700
Soil heat flux ($W \cdot m^{-2}$)	*G*	−110	220
Momentum flux ($kg \cdot m^{-1} \cdot s^{-2}$)	*Tau*	−100	100

Since different input variables have typical values, which vary significantly, all inputs data are normalized to scale between 0 and 1 for easy calculation and prevention of overfitting. The equation is as follows:

$$X_{\mathrm{scaled}} = (x - x_{\min}) / (x_{\max} - x_{\min}), \tag{4}$$

where X_{scaled} is normalized value of input variable, $x_{\max}$ is maximum value of input variable, $x_{\min}$ is minimum value of input variable.

1.4 Architecture of ANN model

Researchers have applied ANN technique to simulate CO_2 flux[6,7,9], but energy fluxes were not used in the neural network design. With the development of inverse method in remote sensing, a neural network capable of correlating energy fluxes to CO_2 fluxes has a potential to be used for spatial mapping of the later using data from remote sensing, and ANN technique is rarely used in grassland and cropland ecosystems. The studies select energy fluxes (net radiation, latent heat, sensible heat, and soil heat flux), air temperature, soil temperature, and soil moisture as input variables, depending on whether to select soil moisture and build two different architectures of ANN model. Architecture of model is indicated in Table 3. The difference between model 1 and model 2 lies in that soil moisture is included in model 1 but not in model 2. The architecture of network is 6(7)-10-1, also input layer have 7 units (model 1) or 6 units (model 2), hidden layer have 10 units, output layer have 1 unit.

Table 3 Architecture of ANN model 1 and model 2

No.	Input variables	Output variables
Model 1	net radiation, sensible heat, latent heat, soil heat flux, air temperature, soil temperature, soil moisture	CO_2 flux
Model 2	net radiation, sensible heat, latent heat, soil heat flux, air temperature, soil temperature	CO_2 flux

1.5 Contributions of input variables in ANN model

As the ANN model is usually regarded as “Black-Box” model, researchers cannot understand the internal-process of phenomenon. But they attempt to understand the relationship between input variables and output variables through different methods, to help researchers optimize the network architecture or study the contribution of input variables, overcoming the disadvantage of ANN model. Gevrey *et al*.[16] have used eight different methods (connect weight, sensitivity analysis, etc.) to study the contribution of input variables. Based on Gevrey *et al*’s study, Julian *et al.*[17] provided more appropriate comparison by using simulation data and Monte Carlo method. Results showed that a connection weight approach using raw input-hidden and hidden-output connection weights in the neural network provided the best methodology for accurately quantifying variable importance. In the study, we have used connect weights method to quantify variable importance. Detailed steps are as follows:

1) Calculating the weight index Q_{ij} of hidden layer neuron j. Consider the neural network with three-layer architecture, the equation is as follows:

$$Q_{ij} = \frac{|W_{ij}| \times |W_{jk}|}{\sum_{i=1}^{n}(|W_{ij}| \times |W_{jk}|)}, \tag{5}$$

where W_{ij} is the weight between input layer and hidden layer, W_{jk} is the weight between hidden layer and output layer, i=1,2…n, n is number of input variables, j=1,2….p, p is number of hidden layer, k=1,2…q, q is number of output layer. In the study, k=1.

2) Calculating the relative important index (RI %) of input variables.

$$RI(\%)_i = \frac{\sum_{j=1}^{p} Q_{ij}}{\sum_{j=1}^{p}\sum_{i=1}^{n} Q_{ij}} \times 100. \tag{6}$$

1.6 Model assessment

The evaluation of the error of training, test and validation dataset made by the neural network is done through the calculation of different error typologies, we have used

Pearson correlation coefficient (r):

$$r = \frac{\sum (y - \mathrm{mean}(y))(\hat{y} - \mathrm{mean}(\hat{y}))}{\sqrt{\sum_p (y - \mathrm{mean}(y))^2 \sum_p (\hat{y} - \mathrm{mean}(\hat{y}))^2}}. \tag{7}$$

root mean squared error (RMSE):

$$\mathrm{RMSE} = \sqrt{\frac{\sum_p (y - \hat{y})^2}{p}}. \tag{8}$$

mean absolute error (MAE):

$$\mathrm{MAE} = \frac{1}{p}\sum_p |y - \hat{y}|, \tag{9}$$

where p is the number of examples, $\hat{y}$ is the predicted values and y is the real values; mean is mean value.

2 Results and discussion

2.1 Analysis of input data

Average diurnal variation of energy fluxes, CO_2 flux, and temperature for the three ecosystems during June—August in 2003 is shown in Fig. 2. In all the three ecosystems, a close correlation between CO_2 flux and net radiation, latent heat, sensible heat, soil heat flux, air temperature, soil temperature is shown. In growing season of the three ecosystems, CO_2 flux value is negative and the dominant source of carbon flux is the nighttime vegetation respiration, therefore, these ecosystems represent “carbon sinks”. During the peak photosynthesis window of the day, plants utilize carbon dioxide, leading to a declining carbon concentration. The energy flux data from the flux towers include the net radiation, latent heat and sensible heat. Attributed to vegetation cover, latent heat is more than sensible heat. Usually, energy flux includes net radiation, sensible heat, latent heat and soil heat flux, and the partitioning of net radiation to sensible heat, latent heat and soil heat flux is highly dependent on albedo and Bowen ratio, so vegetative cover plays a very important role in this process. This makes correlation of energy and carbon fluxes inside ANN very practical.

2.2 Simulation result for cropland, grassland and forest ecosystems

Error (MAE and RMSE) and Pearson correlation coefficient (r) of training, test, validation between real value and predicted value by ANN model in the three different ecosystems are indicated in Table 4, Figs. 3—5.

During training, test and validation, results of model 1 or model 2 indicate that the CO_2 flux modeled from the energy fluxes and temperature demonstrate a good agreement with the observed values.

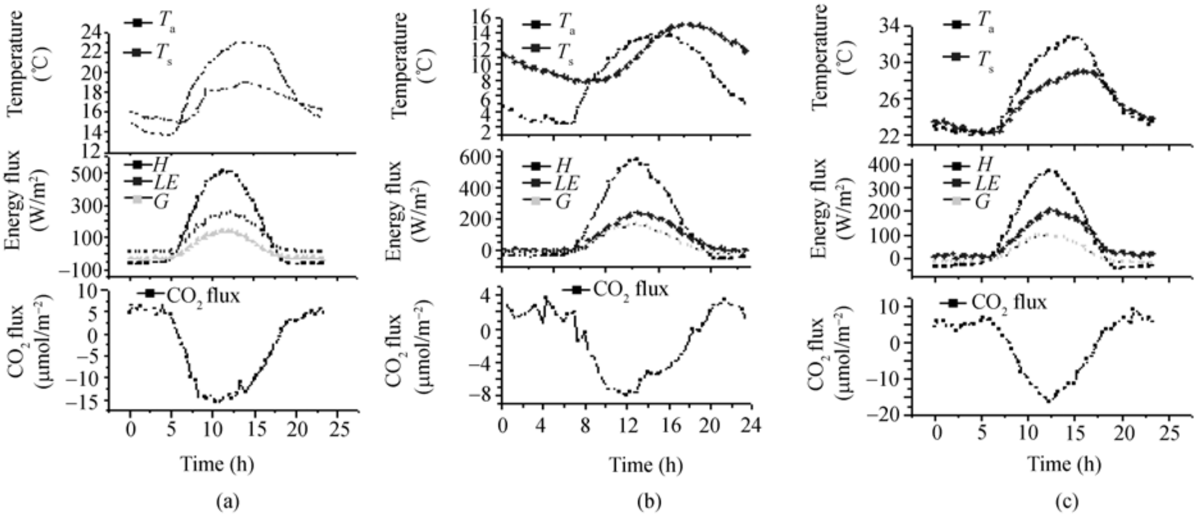

Fig. 2. Average diurnal variation of temperature, energy fluxes, CO_2 flux at the three different ecosystems (June—August, 2003). (a) Forest ecosystem, Changbai Mountains; (b) grassland ecosystem, Haibei; (c) cropland ecosystem, Yucheng.

Table 4 Statistical indices showing the ANN model performance[a)]

	Site name	Changbai Mountains			Haibei			Yucheng		
		Training	Testing	Validation	Training	Testing	Validation	Training	Testing	Validation
	Number	1246	416	416	1138	380	380	1280	428	428
Model 1	R^2	0.863	0.807	0.845	0.808	0.825	0.757	0.867	0.871	0.863
Model 2		0.860	0.807	0.839	0.802	0.821	0.770	0.857	0.856	0.866
Model 1	RMSE	0.0078	0.01193	0.0092	0.0125	0.0116	0.0124	0.0086	0.00954	0.0097
Model 2		0.0080	0.011253	0.0099	0.0129	0.0117	0.0125	0.0092	0.0103	0.0098
Model 1	MAE	2.61	3.04	2.75	1.39	1.38	1.59	3.04	3.14	3.58
Model 2		2.65	3.03	2.89	1.59	1.47	1.63	3.58	3.39	3.60

a) The unit of RMSE and MAE were μmol · m^{-2}.

As to simulation results, the cropland ecosystem is the best one, with R^2 of 0.86, RMS of 0.0086 μmol/m^2 and MAE of 3.04 μmol/m^2. The forest ecosystem is found to be second, with R^2 of 0.84, RMS of 0.012 μmol/m^2 and MAE of 1.59 μmol/m^2. In Haibei, a grassland ecosystem, the results are the worst, with the R^2, RMS and MAE rated as above 0.77, 0.0092 and 2.75 μmol/m^2 respectively. Slim as it is, the difference of simulation result of three ecosystems is perhaps correlated to the number of sample data, which are counted to be 2136, 2078 and 1898 in Yucheng, Changbai and Haibei sites. The reason for Haibei site is that precipitation that occurred in night time reduces the number of sample data in the area.

2.3 The contribution of soil moisture to CO_2 flux in different ecosystems

Soil moisture and soil temperature play a very important role in the amount of soil respiration. Valentini[18] indicated that the inclusion of soil moisture could improve the predictions. In the study, inclusion of soil moisture (model 1) has improved the prediction, though not significantly. Fig. 6 shows that from June to August in 2003, in three different ecosystems, most of soil water content were above 0.22 m^3/m^3, except that in some days in Changbai Mountain. Compared with previous years, Changbai Mountain experienced a drought year, but there was no water stress phenomenon. Therefore, in

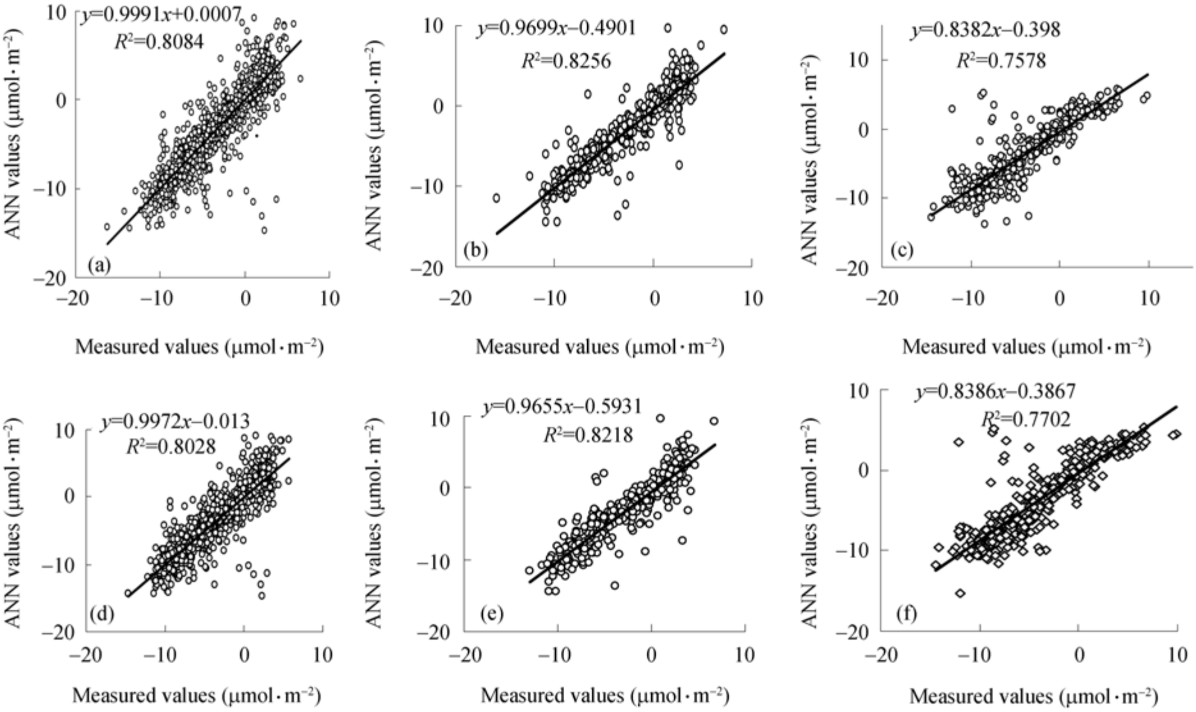

Fig. 3. Measure vs. ANN NEE values for training, testing and validation dataset at Haibei site (grassland ecosystem). Upper: Measure vs. ANN NEE values for 7 input variables (model 1 inclusion of soil moisture). (a) Training dataset; (b) testing dataset; (c) independent validation dataset. Lower: Measure vs. ANN NEE values for 6 input variables (model 2 not inclusion of soil moisture). (a) Training dataset; (b) testing dataset; (c) independent validation dataset.

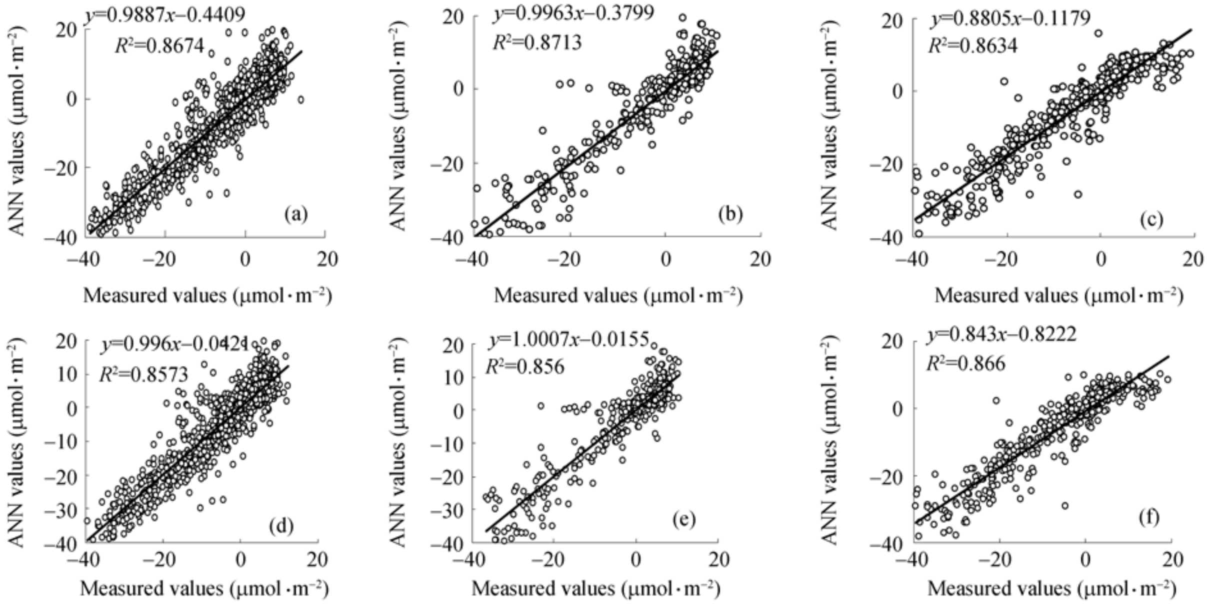

Fig. 4. Measure vs. ANN NEE values for training, testing and validation dataset at Yucheng site (cropland ecosystem). Upper: Measure vs. ANN NEE values for 7 input variables (model 1 inclusion of soil oisture). (a) Training dataset; (b) testing dataset; (c) independent validation dataset. Lower: Measure vs. ANN NEE values for 6 input variables (model 2 not inclusion of soil moisture). (a) Training dataset; (b) testing dataset; (c) independent validation dataset.

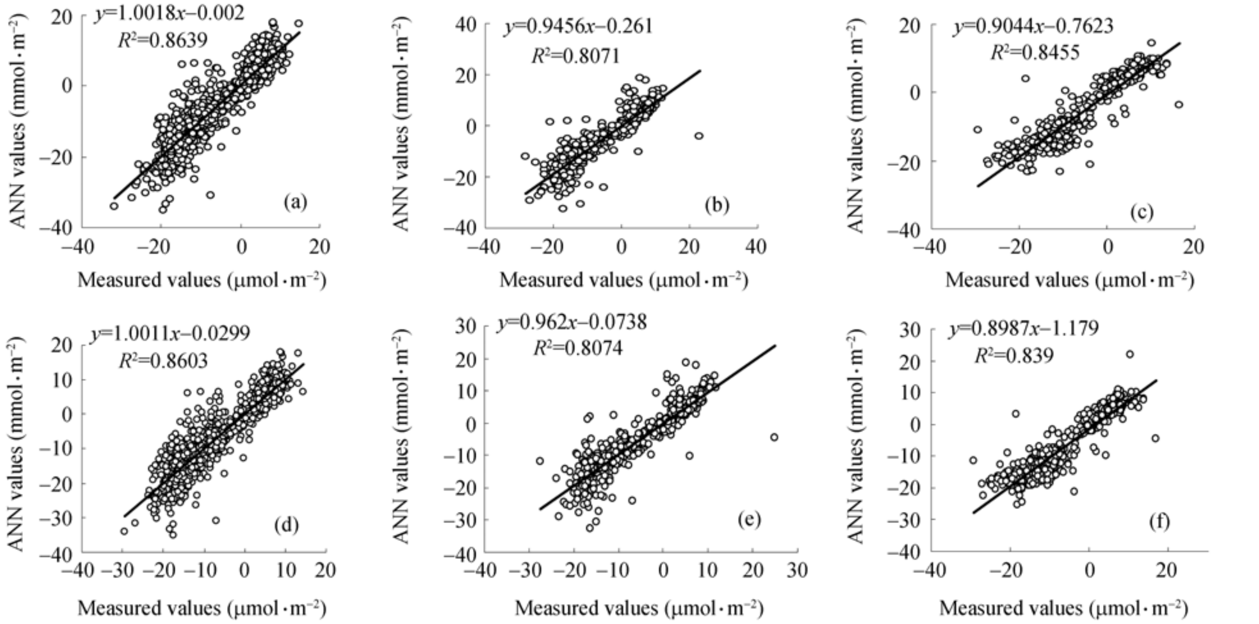

Fig. 5. Measure vs. ANN NEE values for training, testing and validation dataset at Changbai Mountain site (forest ecosystem). Upper: Measure vs. ANN NEE values for 7 input variables (model 1 inclusion of soil moisture). (a) Training dataset; (b) testing dataset; (c) independent validation dataset. Lower: Measure vs. ANN NEE values for 6 input variables (model 2 not inclusion of soil moisture). (a) Training dataset; (b) testing dataset; (c) independent validation dataset.

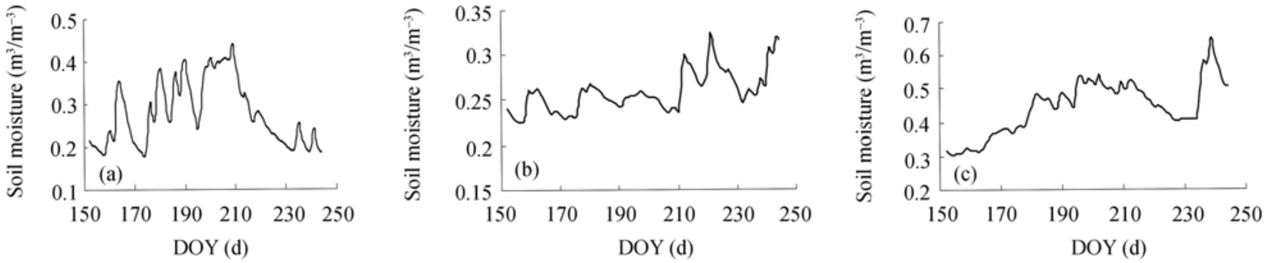

Fig. 6. Dynamics of soil moister in the three ecosystems from June to August in 2003.

the three ecosystems, from June to August, soil moisture has not contributed significantly to NEE, nor can ANN model inclusion of soil moister greatly improve the prediction accuracy.

2.4 The contributions of input variables to NEE

The contribution of input variables to NEE on model 1 and model 2 is shown in Fig. 7. Results show that contribution of input variables to NEE varies greatly in different ecosystems. At Haibei and Changbai Mountain sites, energy fluxes play a more important role than temperature. It perhaps means that from June to August, Haibei (grassland ecosystem) and Changbai Mountain (forest ecosystem) are carbon sinks. As ecosystem photosynthesis exceeds the respiration and temperature is an important contributor in the respiration, the temperature variable is subordinate to other variables. At Haibei site, contribution of latent heat variable is more than sensible heat in energy flux. In Changbai Mountain, however, the situation is opposite. It is correlation between NEE and micrometeorological environment in these sites. The case when Bowen ratio, a ratio of sensible heat versus latent heat, is smaller than 1

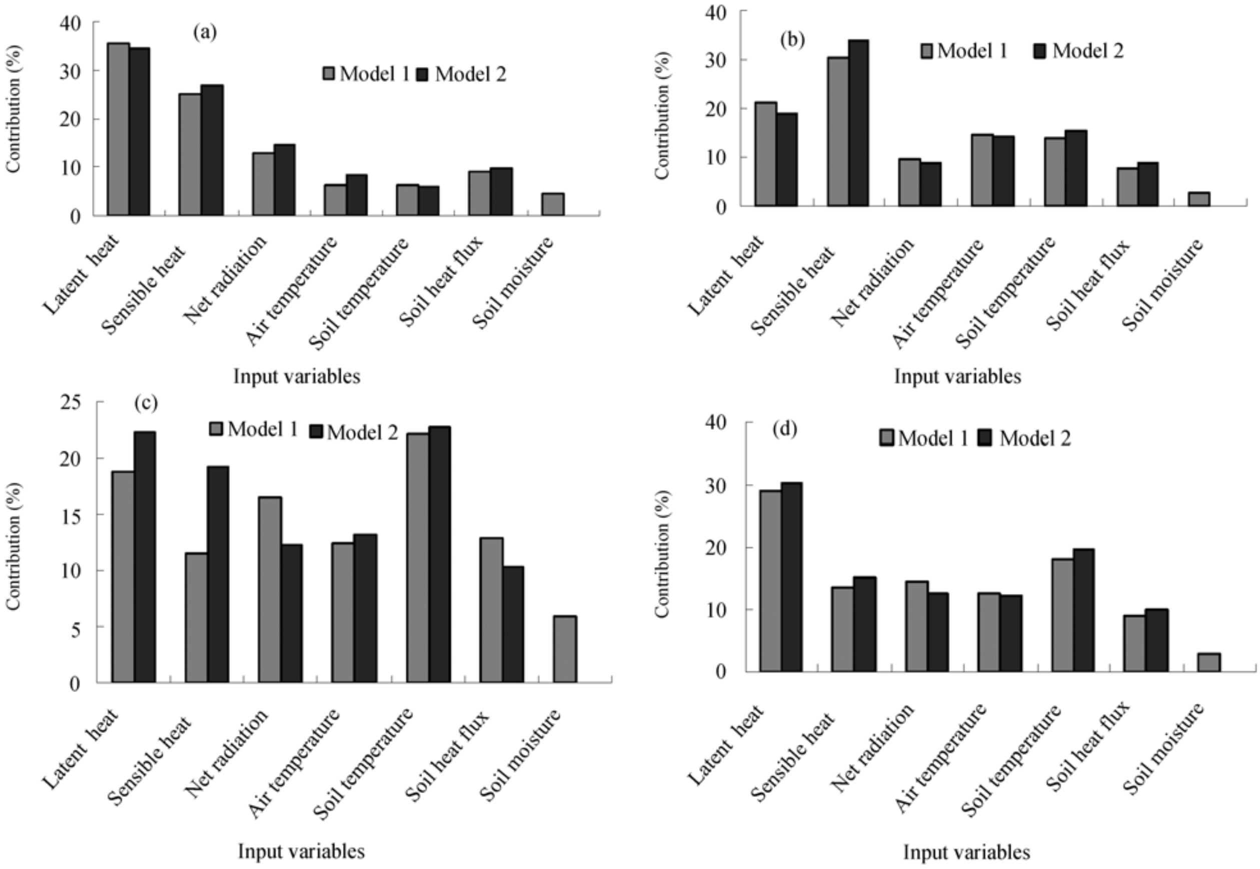

Fig. 7. Contribution of input variables. (a) Haibei; (b) Changabai Mountais; (c) Yucheng (from 15, June to 31, August); (d) Yucheng (from 20, July to 31, August).

shows a wet climate, while Bowen ratio is larger than 1 means a dry climate. This phenomenon is consistent with environmental condition of Haibei and Changbai Mountain sites. At Yucheng site, soil temperature plays a more important role than other input variables. It probably means that from 15, June, when summer maize is just sown without other vegetation, the NEE is dominated by the respiration (nighttime and daytime) and there is no water stress, therefore, the contribution of soil temperature is larger than other variables during the whole growing season of the maize from June to August. Based on this, we simulate the NEE using data from 20, July to 30, August by ANN model. The result is shown in Fig. 7(d). Contribution of latent heat is more than temperature and heat temperature. It is consistent with the fact that moisture is abundant at Yucheng site in 2003. So we can understand the NEE change patterns and corresponding information by means of weight analysis of ANN model.

2.5 Advantage and disadvantage of ANN model

The advantage of ANN model is that it can simulate interaction between input variables and CO_2 flux, train and model input multi-variable sample and its model result is satisfactory without using the complicated mathematical equation. ANN model is especially used to simulate the output/input variables interaction that has not yet been fully understood.

ANN model is generally regarded as an empiristic model without the ability to extrapolate due to its dependence on the inter-structure of training dataset, instead of the understanding of ecosystem process. In the study, we use cross-validation and independent validation to prove that ANN model has some power of extrapolability. ANN model needs more parameters than process model. Only with sufficient samples will the ANN have a power to extrapolate, otherwise it may lead to overfitting. So we need to be careful when using ANN model to extrapolate.

3 Conclusion

The applicability of ANN to carbon flux simulation from other micrometeorological variables was studied for the three different ecosystems (cropland, grassland and forest). The average diurnal fluxes (CO_2 versus energy) and (CO_2 versus temperature, air and soil) variations from three ecosystems show that a close correlation exists among carbon flux and energy fluxes, and carbon and temperature (air and soil). Half-hourly data from June to August in 2003 in the three ecosystems were divided into training, testing and validating, including or excluding soil moisture. Results show that the carbon simulation applied for the three different ecosystems corresponds well with observed flux values, with R^2 all above 0.8.

Though soil moisture and soil temperature have an important role in soil respiration, when there is no water stress, inclusion of soil moisture cannot improve the prediction in the three different ecosystems. The analysis of the contribution of input variables in ANN shows that the ANN is not a black box model, it can tell us about the controlling parameters of NEE in different ecosystems and micrometeorological environment. The results indicate that the ANN is not only a reliable and efficient technique to estimate regional or global CO_2 flux from point measurements and understand the spatiotemporal budget of the CO_2 fluxes, but also can identify the interactions between the CO_2 flux and micrometeorological variables.

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