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Testing the applicability of neural networks as a gap-filling method using CH_4 flux data from high latitude wetlands

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Abstract

Since the advancement in CH_4 gas analyser technology and its applicability to eddy covariance flux measurements, monitoring of CH_4 emissions is becoming more widespread. In order to accurately determine the greenhouse gas balance, high quality gap-free data is required. Currently there is still no consensus on CH_4 gap-filling methods, and methods applied are still study-dependent and often carried out on low resolution daily data.

In the current study, we applied artificial neural networks to six distinctively different CH_4 time series from high latitudes in order to recover missing data points, explained the method and tested its functionality. We discuss the applicability of neural networks in CH_4 flux studies, the advantages and disadvantages of this method, and what information we were able to extract from such models.

In keeping with the principle of parsimony, we included only five standard meteorological variables traditionally measured at CH_4 flux measurement sites. These included drivers such as air and soil temperature, barometric air pressure, solar radiation, and in addition wind direction (indicator of source location). Four fuzzy sets were included representing the time of day. High Pearson correlation coefficients (r) of 0.76–0.93 achieved in the final analysis are indicative for the high performance of neural networks and their applicability as a gap-filling method for CH_4 flux data time series. This novel approach that we showed to be appropriate for CH_4 fluxes is a step towards standardising CH_4 gap-filling protocols.

1 Introduction

Methane is one of the most important long-lived greenhouse gases, second only to CO_2 (IPCC, 2007), with natural wetlands thought to be the biggest individual source (IPCC, 2007; EPA, 2010). Since the advancement in CH_4 gas analyser technology and its applicability to eddy covariance flux measurements (Hendriks et al., 2008;

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Eugster and Plüss, 2010; Dengel et al., 2011; McDermitt et al., 2011; Peltola et al., 2013), monitoring of CH_4 emissions is becoming more widespread in northern regions (Mastepanov et al., 2008; Sachs et al., 2008; Zona et al., 2009; Sturtevant et al., 2012). These measurements contribute to a better understanding of the greenhouse gas balance of the Arctic and subarctic. In order to accurately estimate annual greenhouse gas budgets, time series of high quality gap-free data are required (Falge et al., 2001; Rinne et al., 2007).

Currently there is no consensus on CH_4 gap-filling methods. Several studies (Zona et al., 2009; Gažovič et al., 2010; Sturtevant et al., 2012) did not apply any gap-filling to their CH_4 flux data. Studies where gap-filling was applied were site dependent and often applied to low resolution daily mean values (Hargreaves et al., 2001; Rinne et al., 2007; Riutta et al., 2007; Jackowicz-Korczyński et al., 2010; Long et al., 2010; Tagesson et al., 2012), while Wille et al. (2008); Parmentier et al. (2011) and Forbrich et al. (2012) employed a model in order to recover missing data in their daily, 3 hourly and 30 min mean data, respectively.

Hargreaves et al. (2001), Rinne et al. (2007), Long et al. (2010) and Tagesson et al. (2012) identified a non-linear relationship between CH_4 flux and peat temperature at depths of 0 to 10 cm, 35 cm, and 50 cm in subarctic ecosystems, respectively. During extended periods where no dependency on peat temperature was found, Rinne et al. (2007) and Tagesson et al. (2012) applied a simple interpolation to gap-fill these datasets. In addition, Tagesson et al. (2012) applied an exponential regression between half-hourly CH_4 fluxes and friction velocity measured after the soil was completely frozen. No dependency on water table position was found by the two studies mentioned above. A similarly simple peat temperature relationship with CH_4 emissions was also found by Jackowicz-Korczyński et al. (2010). Wille et al. (2008) and Sachs et al. (2008) found strong relationships between CH_4 flux, friction velocity and soil temperature at a depth of 20 cm and 10 cm, respectively. Some of the above mentioned studies considered nonlinear relationships to gap-fill their daily averaged CH_4 fluxes, while Parmentier et al. (2011) provide a method for gap-filling of higher resolution (3 h)

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data. This method applied a gap-filling model that includes the attenuating effect of atmospheric stability on flux measurements, where methane production was related to soil temperature and water level. Recently Forbrich et al. (2011) tested various models where peat temperatures at various depths, water table level, barometric pressure, and friction velocity were integrated in order to gap-fill their time series. Furthermore, large uncertainties in applied methods do still exist with no common protocol on missing data recovery of CH_4 eddy covariance flux data.

The application of neural networks (Jain et al., 1996; Svozil et al., 1997; Elizondo and Góngora, 2005; Saxén and Pettersson, 2006) for data recovery and gap-filling (Aubinet et al., 2000; Gorban et al., 2002; Papale and Valentini, 2003; Ooba et al., 2006; Moffat et al., 2007; Schmidt et al., 2008) has proven to be a very reliable tool in several scientific disciplines (Gardner and Dorling, 1998, 1999; Lek and Guégan, 1999; Lee and Jeng, 2002; Toptygin et al., 2005). In atmospheric sciences (Gardner and Dorling, 1998; Toptygin et al., 2005; Chattopadhyay and Chattopadhyay, 2008), application of neural networks in forecasting has become a standard application tool. Neural networks have the reputation of being a "black box" where transparency is limited in most cases (Elizondo and Góngora, 2005). This partly results from a neural network's high capacity in training itself where coefficients are distributed through fitted weights and spread across several layers to accurately reproduce a given data set. In the current study, we discuss the applicability of neural networks to gap-fill CH_4 flux data from northern high latitude ecosystems (wet sedge tundra, sedge fen and polygonal tundra), some driver dynamics, the advantages and disadvantages of this method, and what information can be extracted from such a model.

Since CH_4 is the second most potent long-lived greenhouse gas in the atmosphere (IPCC, 2007), it is becoming increasingly important to introduce a method which is capable of dealing with such high resolution data combined with auxiliary measurements, and which is easy to implement across a variety of ecosystems. Regarding Arctic and subarctic regions, it is very important to work with time series where data gaps have been filled using reliable methods in order to accurately determine CH_4 emissions,

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potential annual budgets, and prediction of future emissions under a changing climate (Anisimov, 2007; IPCC, 2007). The datasets introduced in the current study were chosen, as they are showing distinctive differences in their emission patterns and originate from high latitude ecosystems (Fig. 1) to assure the broad applicability of the introduced methods/results.

The aim of the current study is to find a gap-filling tool that is applicable to Arctic and subarctic ecosystems where CH_4 flux data are reported at 30 min/1 h time resolution including a limited number of standard meteorological variables measured at all sites that act as drivers for methane emissions in such dynamic ecosystems. This novel approach in CH_4 studies is a first step towards standardising CH_4 gap-filling and a contribution to standardising CH_4 measurement protocols.

2 Materials and methods

2.1 Methane flux and meteorological data

The CH_4 eddy covariance flux data used in the current study originates from five distinctively different northern ecosystems (Fig. 1): the subarctic sites of Stordalen (68°20′ N, 19°03′ E), a mixed mire (Johansson et al., 2006) and Lompolojänkkä a nutrient-rich sedge fen located in the aapa mire region of north-western Finland (67°59′ N, 24°12′ E) (Aurela et al., 2009), and the tundra sites underlain by permanent permafrost: Samoylov Island in the southern central Lena River Delta (72°22′ N, 126°30′ E) (Sachs et al., 2008, 2010), Kytalyk (70°49′ N, 147°29′ E) (Parmentier et al., 2011) and Barrow a wet sedge tundra in the northern part of the Arctic Coastal Plain (71°17′ N, 156°36′ W) (Zona et al., 2009).

The CH_4 fluxes were measured by the eddy covariance (EC) method (Baldocchi, 2003). Instrumentation used in these six studies were the three-dimensional sonic anemometer R3-50 (Gill Instruments Ltd., Lymington, Hampshire, England) coupled with a closed path Fast Greenhouse Gas Analyser (FGGA, Los Gatos Research,

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Mountain View, California, USA) in Stordalen; the USA-1 (METEK, Elmshorn, Germany) three-axis sonic anemometer/thermometer and the closed-path DLT-100 fast response CH_4 gas analyser (Los Gatos Research, Mountain View, California, USA) in Lompolojänkkä, and the three-dimensional Solent R3 sonic anemometer (Gill Instruments Ltd., Lymington, Hampshire, UK) and the TGA 100 tunable diode laser spectrometer (Campbell Scientific Ltd., USA) in the Lena River Delta. At the Kytalyk site, a three-dimensional Solent R3-50 sonic anemometer (Gill Instruments Ltd., Lymington, Hampshire, UK) and a closed-path DLT-100 fast response CH4 gas analyser (Los Gatos Research, Mountain View, California, USA) were used in both years, while a WindMasterPro sonic anemometer (Gill Instruments Ltd., Lymington, Hampshire, UK) and the closed-path DLT-100 fast response CH4 gas analyser (Los Gatos Research, Mountain View, California, USA) was used in Barrow.

The reader is advised to consult Jackowitz-Korczynski et al. (2010), Aurela et al. (2009), Sachs et al. (2008), Parmentier et al. (2011) and Zona et al. (2009), for more details about the sites, measurements and further instrumentation. All five sites recorded standard meteorological variables, such as air temperature, solar radiation, soil temperature at various depths, wind speed and wind direction. CH_4 eddy covariance flux data from Lompolojänkkä and Barrow were u* filtered, while the data from Kytalyk was filtered for occurrences of high atmospheric stability, prior to including in the current study. Data introduced in the current study was not previously gap-filled at 30 min/1 h (Lena River Delta) resolution.

2.2 Artificial neural networks

The topology of a simple multi-layer feed-forward neural network includes non-linear elements (neurons) that are arranged in successive layers (Fig. 2). The information flows unidirectionally, from the input (covariates) layer to the output (response) layer, through the hidden layer(s) (Jain et al., 1996; Svozil et al., 1997; Elizondo and Góngora, 2005; Saxén and Pettersson, 2006).

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In the initial phase, a set of input and target data is used for training and presented to the network many times. A training set should have sufficient data to be representative of the overall dataset. Training is carried out by constantly adjusting the fitted weights so that the network output matches the target data. During the testing phase, a new set of input data is fed into the network and the desired output compared with those predicted by the network. The agreement or disagreement of these two data sets is an indication of the performance of the neural network model. A chosen error function measures the difference between predicted and observed output.

One of the drawbacks of neural networks is the non-uniqueness of the global minimum (Hammerstrom, 1993; Nguyen and Chan, 2004) which changes, as each training run achieves different weights and results (it is important to find a set of weights that processes data accurately enough for the application). Another issue with neural networks is the possibility of under- or over-fitting of networks (Hansen and Salamon, 1990; Jain et al., 1996; Svozil et al., 1997). This can happen when data presented in the training phase is not representative enough for the entire observation span, not the correct number of hidden layers or neurons, if the global minimum is overshot or when the network learns the training pattern well but is underperforming in the testing phase (poor generalisation) (Jain et al., 1996; Gardner and Dorling, 1998; Nguyen and Chan, 2004; Wang et al., 2005; Saxén and Pettersson, 2006; Stathakis, 2009). To avoid this from happening, one can remove redundant input data (Gunaratnam et al., 2003; Saxén and Pettersson, 2006) and use the appropriate generalisation such as early stopping or cross-validation (Hansen and Salamon, 1990; Amari et al., 1997; Svozil et al., 1997; Wang et al., 2005), which has been implemented in the current study.

2.3 Pre-processing of data

Recently, several studies (Zhang and Qi, 2005; Klevecka and Lelis, 2009) pointed out an ongoing debate on whether data should be de-seasonalised prior to applying neural networks. Nelson et al. (1999) showed better results for de-seasonalised time series, while others (Sharda and Patil, 1992; Franses and Draisma, 1997) found that neural

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networks are able to model seasonality directly and prior de-seasonalisation is not necessary. Regarding gap-filling of atmospheric trace gas fluxes (Wijk and Bouten, 1999; Aubinet et al., 2000; Carrara et al., 2003; Papale and Valentini, 2003; Ryan et al., 2004; Ooba et al., 2006; Schmidt et al., 2008), no de-seasonalisation of data was carried out prior to applying neural networks. In the current study, we decided to follow this method, so no de-seasonalisation of data was carried out.

As has been mentioned above, we are dealing with seasonal and diurnal data that experience regular and predictable changes. In order to add this seasonal and diurnal effect to their neural network, Papale and Valentini (2003) added several fuzzy sets reflecting the diurnal and seasonal variation to reduce the linear cumulative numerical weight of time in relation to other variables. Adding this type of input to neural networks does not always increase the neural network performance, and has been shown by Schmidt et al. (2008) to have sometimes little effect. We have decided to follow the method by Papale and Valentini (2003) and have included four fuzzy sets representing the diurnal effect but not the seasonal. This has been excluded as none of the datasets were long enough. We kept the model simple following the principle of parsimony (Beck, 1943; Bugmann and Martin, 1995). The predictive ability of a model initially increases with complexity but they do also have the tendency to decline once a model becomes too complicated (Bugmann and Martin, 1995).

The meteorological, soil, and CH_4 flux data as well as the fuzzy data sets consist of different magnitudes and units. In order to generalise the data, we have scaled all data from 0 to 1 as has been previously applied by Wijk and Bouten (1999), Papale and Valentini (2003) and Nguyen and Chan (2004). Furthermore, the range between 0 and 1 is also necessary as we are applying a sigmoid activation function (Cybenko, 1989), which has a range of 0 to 1. By scaling the data that we are feeding into the network, all data is being treated equally and weights can be distributed evenly. A sigmoid function was also used in the output layer (Fig. 2), as has been previously applied by Papale and Valentini (2003).

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2.4 Statistical analysis

In order to examine all input variables and their effect on methane fluxes, we applied a simple stepwise regression (a combination of backward elimination and forward selection) in R (R Development Core Team, 2012), in order to search for the best predictors or combinations of predictors from among all available 30 min and 1 h (Lena River Delta) resolution data. Thereafter, we chose those variables that appeared important and available in all datasets. Following the principle of parsimony, and by keeping the model simple, we decided on fife meteorological variables (see Fig. 2) and four fuzzy sets representing morning (FL M), afternoon (FL A), evening (FL E) and night (FL N) (Fig. 2). This selection helped to prune the network by avoiding insignificant input data (Gunaratnam et al., 2003; Saxén and Pettersson, 2006). Furthermore it did help to standardise the method and make it applicable to all six different datasets in the same way. Adding u* as an input variable in the current study would lead to uncertainties, as u* filtered data do not provide the information necessary for the network to train and learn such conditions in order to predict CH_4 fluxes occurring under similar conditions. Furthermore, precipitation and water table depths, which can also act as CH_4 drivers (Whalen and Reeburgh, 1992; Roulet et al., 1992; Christensen, 1993), were excluded in the current study, as their resolution is often of a different scale, and can have a lagged effect on CH_4 emissions (Bubier et al., 1995).

In order to verify these five drivers, we applied a simple generalised additive model (GAM) (Hastie and Tibshirani, 1986; Wood, 2001), to each of the sites, commonly used in ecological research. They are models where a relationship between the response variable and explanatory variables is established. A smoothing function is applied, where each predictor variable is separated into sections and a polynomial function is fitted (Hastie and Tibshirani, 1986; Wood, 2001; Guisan et al., 2002). The confidence interval (distributed density) in each GAM figure (bottom part) is an indication of the relationship between the predictor and the response variable. On the one hand such models are rarely used as they are difficult to interpret since no parameter values are

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retuned. On the other hand, such models are very good for prediction and explanatory analysis in estimating the functional nature of a response. Such a model does improve our understanding of the dynamics of CH_4 emissions and the respective meteorological drivers. Furthermore, such models combined with tree models (interactions between the explanatory variables), can visualise precise dynamics at each site. Figure 3 (a–c) illustrate both types of models for each of the six datasets. The longer the branch of a tree, the greater the deviance explained. The values at the end of the branches are the mean CH_4 fluxes in nmol $m^{-2} s^{-1}$. Both models were performed using R (R Development Core Team, 2012).

In order to validate the performance of each network we estimated the mean Pearson correlation coefficient (r) (at 95 % confidence level) as a goodness of fit indicator of the measured and predicted fluxes during the training and testing/validation phase. A further error function applied is the simple root mean square error (RMSE) to indicate the range of the error for each scenario, each site and across sites.

2.5 Applying artificial neural networks to data

Introducing the neural network topology (Fig. 2) used in the current study, input variables (left side of the network) are fed into the network with weights fitted and spread across the two layers with information flowing unidirectionally (grey arrows) to the 4 nodes (marked as circles) within the hidden layer, where a bias (offset) (marked with "1") is added.

In this case, the underlying function is simply written as:

$$o = f\left(b + \sum_i w_i x_i\right) \quad (1)$$

where x_i represents the input variables ($x_1, \ldots, x_9$ – in our case), w_i denotes the fitted weights ($w_1, \ldots, w_4$ – for each input variable) and b denotes the bias (or offset) that is added to the weighted sum ($\sum_i w_i x_i$) prior to applying the sigmoid activation function (f), leading further to the next layer, where a new set of weights are distributed,

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together with a bias and the sigmoid activation function before making an estimation of the output values. These output values also have a range of 0 to 1 which were then rescaled to their appropriate unit (nmol $m^{-2} s^{-1}$).

In order to select the training data set, several choices were traditionally available: choosing blocks of data or choosing random data rows of complete data pairs (input variables and target data). Using non-continuous data sets for training is a common approach (Moffat et al., 2007; Schmidt et al., 2008). As we are testing artificial neural networks as a gap-filling method for CH_4 eddy covariance flux data, we utilised the artificial gap length scenarios introduced in Moffat et al. (2007, Appendix A) and applied them to all six datasets. We have chosen three scenarios per gap length (Figs. 4 and 5). These gap lengths represented very short gaps (*v*) of random 30 min values; short gaps (*s*) of random 4 h gaps, medium (*m*) of 1.5 days, long (*l*) of 12 full days and a mixed scenario (*x*), representing a mix of the above mentioned gap lengths. There were cases where artificial gap data points coincided with already existing gaps, resulting in a non-uniform length of testing data sets (artificial gaps). Nevertheless, each scenario extended the already existing gaps by a further 8–14 %. The artificial gap scenarios introduced in Moffat et al. (2007) are for 30 min resolution files which were adjusted for the Lena River Delta dataset, where a 30 min artificial gap was applied to the respective hour value.

The mixed scenario, which represents the most realistic gap scenario in flux data, was then chosen to be used in order to gap-fill the existing measured methane data. All complete data pairs (meteorological and CH_4 data), excluding those 30 min values (or 1 h in the case of the Lena River Delta dataset) coinciding with created artificial gaps, were used for training (~ 90 % of data). Those data rows coinciding with artificial gap values were then used for testing (~ 10 % of data) (Figs. 4 and 5).

Several learning algorithms are available for neural network training; in the current study we applied the resilient backpropagation algorithm (Riedmiller, 1993; Riedmiller and Braun, 1994). It is a first-order optimization algorithm that acts on each weight separately. It modifies the weights in order to find a local minimum of the error function.

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The weights are modified going in the opposite direction of the partial derivatives until a local minimum is reached, leading to an efficient and transparent adaptation process (Riedmiller and Braun, 1993; Günther and Fritsch, 2010). In order to test the network's performance, various error functions can be applied. We chose the sum of squared errors (SSE) and assembled the neural network by implementing the neuralnet package (Fritsch et al., 2010; Günther and Fritsch, 2010) in R Statistical Language (R Development Core Team, 2012) and modifying it accordingly to suit our purposes (adjustment of the learning rate, maximum number of iterations and threshold value for the partial derivatives of the error function (early stopping)).

There is currently no consensus in the scientific community on the number of neurons that should be used (Svozil et al., 1997; Saxén and Pettersson, 2006; Stathakis, 2009) when applying neural networks to data series. In order to apply the appropriate number of neurons, 25 repetitions were run for a selection of neurons (1–12) to help in choosing the appropriate number of neurons (Järvi et al., 2012) within the hidden layer for the final process.

One of the advantages of applying the neuralnet package mentioned above is the possibility to choose an integer specifying the threshold for the partial derivatives of the error function (summed square error) as a stopping criteria (Günther and Fritsch, 2010) that should be achieved during the training phase, along with the maximum number of iterations (epochs) the network should run in order to fulfil our requirements (convergence of the network and finding the local minimum).

Once we were satisfied with the performance of the networks (no further improvement could be realised in terms of goodness of fit), and their ability to predict relatively accurate CH_4 flux values (see Pearson's correlation coefficient (r) and the root mean square error (RMSE) values achieved when testing the trained network in Figs. 4–6, respectively), we re-introduced the entire dataset of gap-free input variables to the networks in order to estimate flux values for those time periods where CH_4 flux values were missing.

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3 Results

We applied artificial neural networks to six different CH_4 flux datasets originating from Arctic regions of Scandinavia, Siberia and Alaska. The input variables (listed in Fig. 2) were air temperature (Air T), soil temperature at the depth of 10 cm (Soil T), wind direction (WD), Solar radiation (Sol rad, substituted with photosynthetic active radiation where not available), barometric air pressure (Air P) and the fuzzy transformation of the time of day represented by the four time periods morning (FL M), afternoon (FL A), evening (FL E) and night (FL N).

The results from the generalised additive model and the respective tree model in Fig. 3 (a–c), visualise the dynamics of CH_4 fluxes at each site. Stordalen (Fig. 3a) and Kytalyk (Fig. 3b, c) show distinctive wind direction dependent fluxes. Stordalen is located on the shores of Villasjön Lake, while Kytalyk is located in a heterogeneous polygonal tundra environment. In Lompolöjänkkä (Fig. 3a) the highest mean fluxes were observed when soil temperature was above 13.5 °C and barometric air pressure below 974 hPa while in Barrow in Alaska (Fig. 3c), results show the significance of air temperature up to 15 °C and north-easterly wind directions, shown by the densely distributed confidence intervals, as well as all the other variables. The respective tree model makes it possible to interpret these dynamics further by suggesting that the highest mean CH_4 fluxes occurred when (in this case) photosynthetic active radiation was above 711 $\mu mol\, m^{-2}\, s^{-1}$, when soil temperature was above 4.42 °C, and air temperature above 10 °C.

For each neuron applied, Fig. 4 shows the distribution of the mean Pearson's correlation coefficient for all runs and gap scenarios in black and the results from the training step in grey. Their training distribution shows an increase in coefficient value with each added neuron, while some of the training results show no improvement with increase in neurons added. The scatter shows that from 4 neurons onwards no real improvement is visible, be it for the short, long or mixed gap length scenario. This is also confirmed by the lack of statistical significance at the 95 % confidence level beyond 4 neurons.

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Figure 5 illustrates the achieved root mean square error (RMSE) values for the training (in black) and testing (in grey) datasets for each scenario for the respective applied neurons. Here again, no improvement is visible beyond 4 neurons, leading to the assumption that 4 neurons were ideal within the hidden layer to be included in the final process where the entire dataset was applied in order to gap fill missing CH_4 values in all six datasets.

In order to visualise the performance of the applied neural networks, we illustrated the goodness of fit of the predicted and actually measured CH_4 flux data for all six datasets showing their distribution along the 1 : 1 regression line in Fig. 6 with little scatter in some of the datasets. High Pearson correlation coefficients of 0.80–0.92 were achieved during the training phase, while values of 0.76–0.93 were achieved during the testing phase.

4 Discussion

Artificial neural networks that have previously been successfully implemented as a gap-filling method (Falge et al., 2001; Moffat et al., 2007) for carbon dioxide flux time series (Aubinet et al., 2000; Carrara et al., 2003; Papale and Valentini, 2003; Schmidt et al., 2008) have been described as a robust, reliable and versatile tool. Nevertheless, their application is time consuming, particularly in finding the appropriate input variables, the appropriate number of hidden layers, and neurons/nodes within these layers, as well as the choice of training and testing/validation datasets (data rows). Furthermore, the global minimum (Hammerstrom, 1993; Nguyen and Chan, 2004) is not unique, and changes with each training run because every training run achieves different fitted weights and results (it is important to find a set of weights that processes data accurately enough for the application).

In the current study, we tested the applicability of neural networks as a gap-filling tool for methane flux data and also made an attempt to standardise the method by including the same input variables for all datasets and using the same number of neurons within

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the hidden layer for each data scenario. In order to test their applicability, we applied the method to various ecosystems by including six distinctively different datasets from high latitudes, one showing diurnal and seasonal variation, two possibly only diurnal, one only seasonal while a fifth data set does not show any diurnal or seasonal variation. The sixth dataset (Stordalen) reflected its position on the shores of Villasjön Lake in its emission patterns.

The chosen input variables (four commonly recorded meteorological parameters that act as CH_4 drivers and wind direction) as well as four fuzzy sets representing time of day appear to be the right choice. Figure 3 (a–c) highlight the complex interaction and dependency of CH_4 fluxes on these drivers. Reducing the number of chosen input variables any further would not comply with the principle of parsimony anymore, of keeping a model simple but not too simple, leading to an underperformance of the network as predicted fluxes did not reach the full range which means the networks were underestimating the fluxes. The chosen meteorological variables included in the current study belong to the main drivers as shown in previous studies (see Introduction part). Hydrological properties, such as precipitation and water table depths, can sometimes have a lagged effect on methane emissions (Bubier et al., 1995) and are not always recorded, or not recorded with the same time resolution as the CH_4 fluxes.

Some of the Pearson correlation coefficients achieved in the current study appear low (Figs. 4 and 6), compared to those achieved for CO_2 fluxes when applying the same method (Moffat et al., 2007). Much higher correlation coefficients ($r > 0.95$) were achieved in the current study when comparing trained data versus actual measured data, but resulted frequently in no acceptable values ($r < 0.70$) during the testing/validation stage of the analysis. Outliers were introduced in places where there were no high or low fluxes. Such results also indicate that the global minimum was overshot and that the network did not converge (see extremely low values in Fig. 4 and high error values in Fig. 5). RMSE error values are also indicative for an overfitting of the model as error values of the training stage are declining while those of the testing/validation stage are rising. Such results could also be due to existing and gap

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scenario data distribution, as artificial gaps coincided with existing gaps, reducing the number of test data points. None of the long gaps included an entire 12 days period that could have been used as a classical "long gap" test data set, as introduced in Moffat et al. (2007). Furthermore it is to be expected that predicting CH_4 emission events is more complex than predicting CO_2 fluxes that undergo a regularity and predictability in respiration or CO_2 uptake, respectively.

Figure 4 (Lena River Delta) displays the lowest mean correlation coefficient values. These values indicated that some runs did not converge, thus resulting in such low mean values. Simultaneously the RMSE values appeared much lower than those from other sites. The extreme discrepancy in case of the Lena River Delta results are due to low CH_4 fluxes recorded at the site with few significant emission events resulting in higher CH_4 fluxes. By increasing the number of runs or discarding iterations that did not converge, this correlation coefficient could be increased in the final analysis (Fig. 6, Lena River Delta). Furthermore the correlation coefficient values for the tested datasets (Lena River Delta and Barrow) showed higher values than the training datasets. This could be due to the fact that Barrow experienced a diurnal trend and the data composing the test dataset did not include any specific events. In case of Lena River Delta the artificial gaps included 2 little events that the network was capable to predict, having learned about such events from similar conditions during the training phase.

Two other important aspects in the current study are the length of the time series, and thus consequently the sufficiency of available training data, and secondly the gap length in the existing time series. Time series vary between 15 days (Kytalyk, 2008) and 181 days (Lompolojänkkä), with Lompolojänkkä having the highest proportion of gaps in the CH_4 fluxes. We could show that the method we introduced in the current study is applicable to short and longer time series. However, none of the time series included in the current study were gap free or included an entire year's worth of data. Therefore, no bias error to indicate the bias induced on the annual sums/budgets, as referred to by Moffat et al. (2007), was calculated.

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Nevertheless, neural networks show excellent performance (Figs. 4–6), which proves that this standardised method is easy to be implemented and applicable to many different ecosystems in the northern latitudes (Fig. 1). We have reliably reproduced and predicted methane fluxes in a way that can be used as a substitute for missing values. This substitute showed a seamless fit into the original dataset where CH_4 data had to be discarded, or was not collected in the first place due to instrument failure. We find artificial neural networks to be recommendable as a reliable and robust gap-filling method for high resolution CH_4 flux data originating from various ecosystems as estimated annual budgets rely on accurate gap-free or gap-filled data.

5 Challenges and recommendations

A peculiar characteristic of CH_4 is their higher emission variability than CO_2 fluxes, often connected to specific events such as those visible in the Lena River Delta dataset. In our case, the network was able to reproduce these events (Fig. 6). In case such events are triggered by other drivers or physical forcing (not included as input variables in neural networks), predicted values do diverge from the actually measured values. Precipitation and water table depth can have a lagged effect on CH_4 fluxes (Bubier et al., 1995) with each rain event being different in intensity and length. The same can be said of water table depths whose rise and fall are not equally predictable after each such event. In addition further uncertainties in predicting/estimating accurate CH_4 emissions do exist regarding the insufficiently understood "pressure pumping effect" (Zamolodchikov et al., 2003) and friction velocity (u^* correction), a parameter known to act as a driver for CH_4 emissions but is also used as a filtering criterion for low turbulence, both affecting methane emissions. These factors might have an influence on how far neural networks are reproducing and predicting CH_4 fluxes accurately.

In order to evaluate, carry out and apply standardised CH_4 flux measurements, data post-processing and gap-filling methods in the future, standardised protocols and required auxiliary measurements are needed to be implemented. First steps towards

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such procedures have already been initiated during the international ESF explanatory (Germany, April 2012) and FLUXNET CH_4 (Finland, September 2012) workshops.

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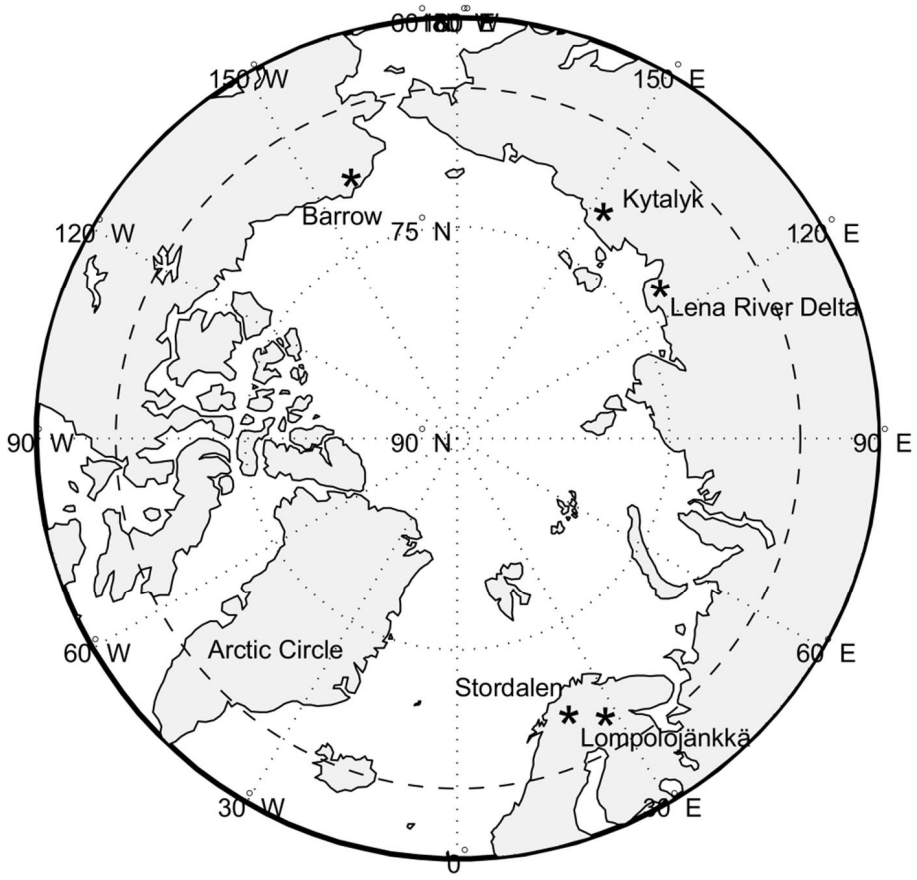

Fig. 1. Map of the Arctic and subarctic region, with Stordalen (Sweden), Lompolojänkkä (Finland) both Siberian sites of the Lena River Delta and Kytalyk in Russia and Barrow (Alaska) marked with an asterisk (*) at their respective location.

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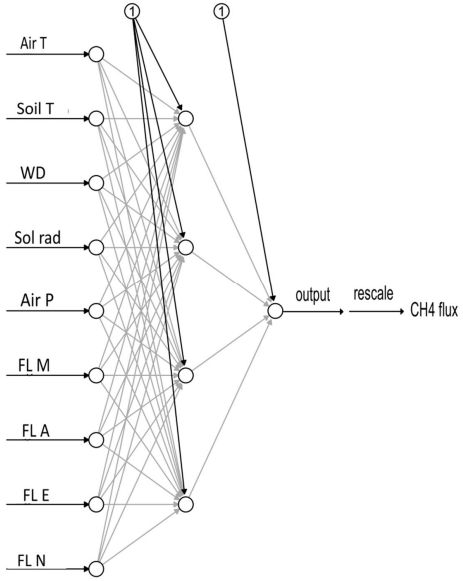

Fig. 2. The architecture of the neural network topology used in the current study. Input variables (left side of the network) are fed into the network with weights fitted (along grey arrows) with information flowing unidirectionally to the nodes (marked as circles) within the hidden layer, where a bias (offset) (marked with "1") is added (along black arrows). Here a sigmoid function (activation function) is applied to the weighted sum, leading further to the next layer, the "output" layer where a new set of weights is distributed, together with a bias and the sigmoid activation function before making an estimate for the output value. As the output still has a range of 0 to 1, it is rescaled prior to replacing missing data values. Actual fitted weights and biases are removed from the graph for clarity. The input variables listed are: air temperature (Air T), soil temperature at the depth of 10 cm (Soil T), wind direction (WD), solar radiation (Sol rad, substituted with photosynthetic active radiation where not available), barometric air pressure (Air P) and the fuzzy transformation of the time of day represented by the four time periods morning (FL M), afternoon (FL A), evening (FL E) and night (FL N).

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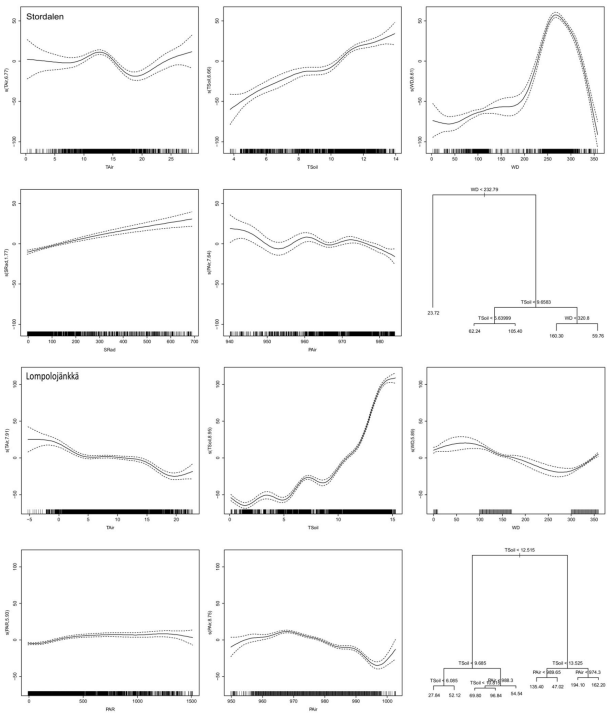

Fig. 3a. Overview of the generalised additive model outcome as well as the representative tree model applied to all 6 datasets. Results are indicative for a dependency of the CH_4 fluxes/emissions on the included driver parameters. Y-axis labels indicate the smooth function (parameter used) and how many degrees of freedom the term has. The dashed lines represent the 2 standard errors above and below the smooth function estimate, roughly the 95 % confident limit. The longer the branch of a tree, the greater the deviance explained. The values at the end of the branches are the mean CH_4 fluxes in nmol m^{-2} s^{-1}.

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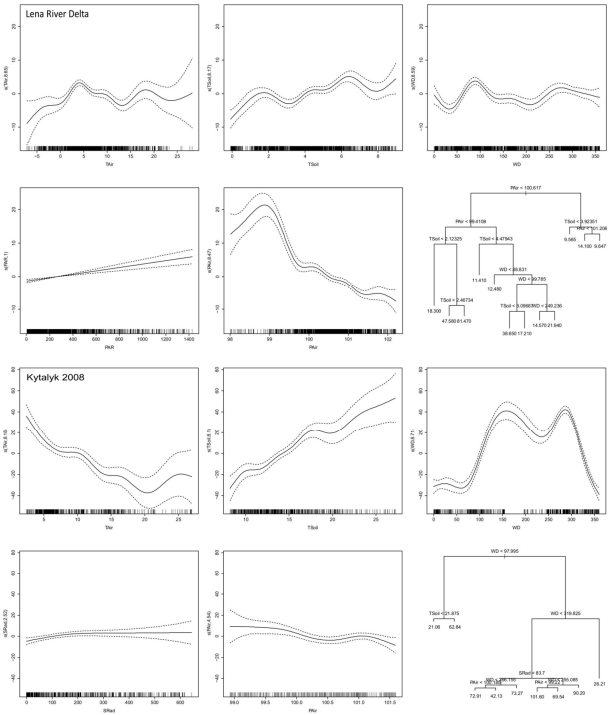

Fig. 3b. Overview of the generalised additive model outcome as well as the representative tree model applied to all 6 datasets. Results are indicative for a dependency of the CH_4 fluxes/emissions on the included driver parameters. Y-axis labels indicate the smooth function (parameter used) and how many degrees of freedom the term has. The dashed lines represent the 2 standard errors above and below the smooth function estimate, roughly the 95 % confident limit. The longer the branch of a tree, the greater the deviance explained. The values at the end of the branches are the mean CH_4 fluxes in nmol m^{-2} s^{-1}.

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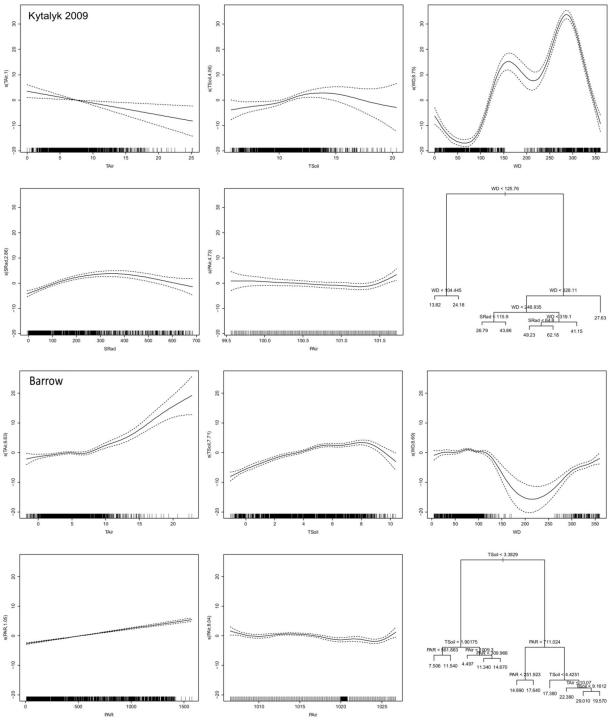

Fig. 3c. Overview of the generalised additive model outcome as well as the representative tree model applied to all 6 datasets. Results are indicative for a dependency of the CH_4 fluxes/emissions on the included driver parameters. Y-axis labels indicate the smooth function (parameter used) and how many degrees of freedom the term has. The dashed lines represent the 2 standard errors above and below the smooth function estimate, roughly the 95 % confident limit. The longer the branch of a tree, the greater the deviance explained. The values at the end of the branches are the mean CH_4 fluxes in nmol m^{-2} s^{-1}.

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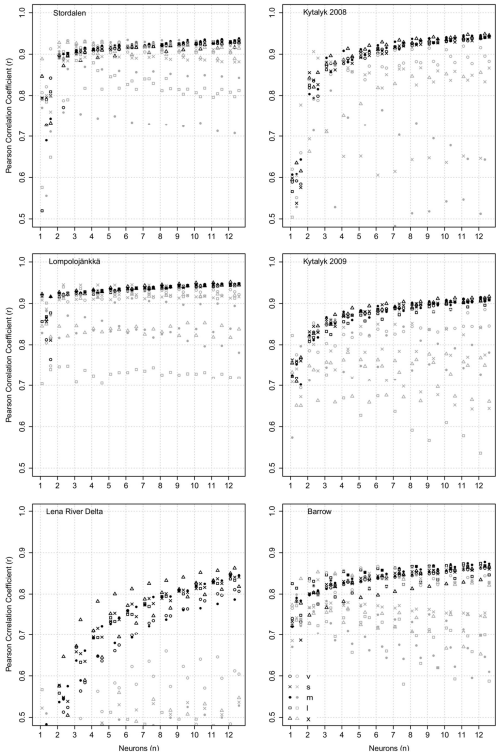

Fig. 4. Output from several neural network iterations. Shown in black is the mean Pearson correlation coefficient achieved for the training dataset for each scenario and for each number of applied neurons (within the hidden layer) and in grey the achieved coefficients for the testing (artificial gaps) dataset. Circles represent very short (*v*) gaps of random 30 min values; crosses short gaps (*s*) of random 4 h gaps, full circles medium (*m*) of 1.5 days, squares long (*l*) of 12 full days and as triangles mixed scenarios (*x*), representing a mix of the above mentioned gap lengths.

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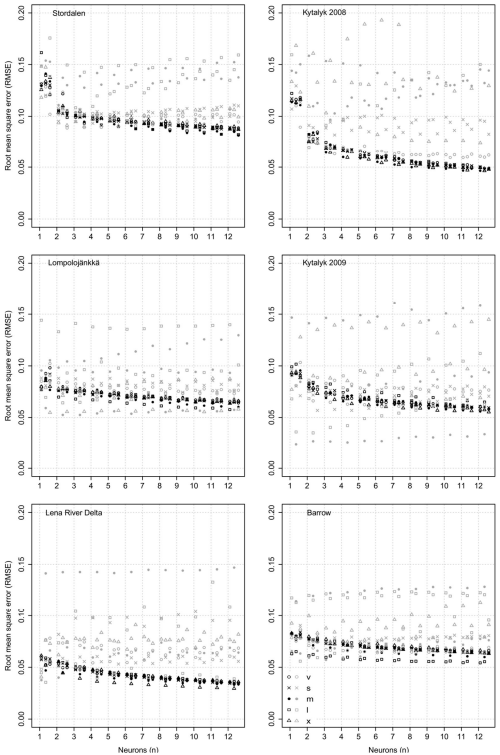

Fig. 5. Output from several neural network iterations. Shown in black are the root mean square error values achieved for the training dataset for each scenario and for each number of applied neurons (within the hidden layer) and in grey the achieved error values for the testing (artificial gaps) dataset. Circles represent very short (*v*) gaps of random 30 min values; crosses short gaps (*s*) of random 4 h gaps, full circles medium (*m*) of 1.5 days, squares long (*l*) of 12 full days and as triangles mixed scenarios (*x*), representing a mix of the above mentioned gap lengths.

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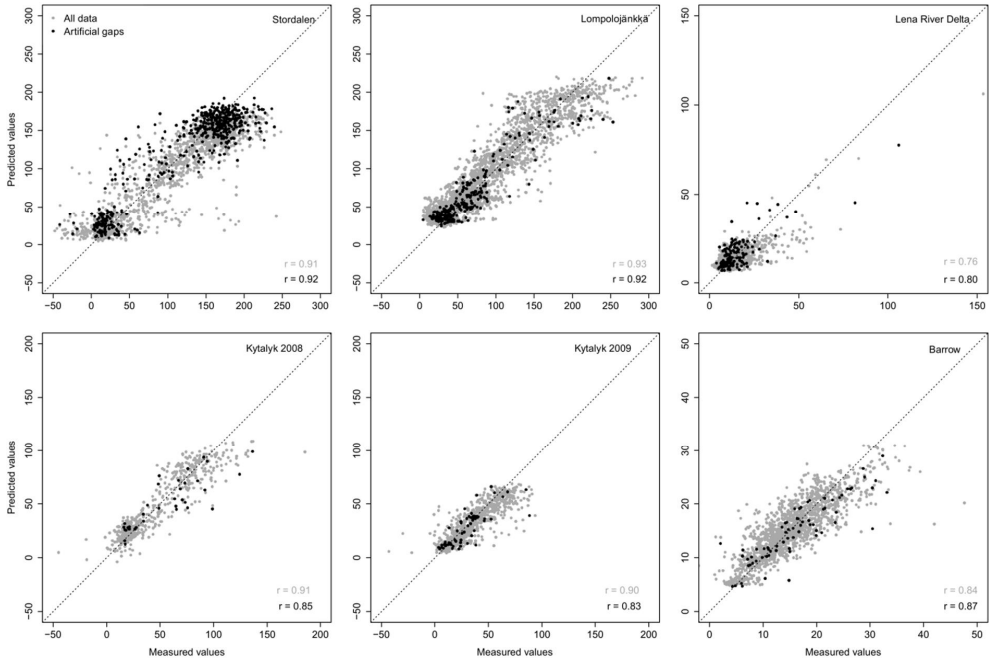

Fig. 6. Scatter plots showing the distribution of the actually measured CH_4 flux values against the mean predicted CH_4 values for all six datasets, and their distribution along the 1 : 1 regression line. All units are in nmol m^{-2} s^{-1}.There is some scatter visible at some sites indicating that the networks did over- or underestimate fluxes at times. The goodness of fit (r) for all six sites was between 0.80–0.92 and 0.76–0.93 for the training and testing datasets, respectively.

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