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Using an extended Kalman filter learning algorithm for feed-forward neural networks to describe tracer correlations

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Abstract

In this study a new extended Kalman filter (EKF) learning algorithm for feed-forward neural networks (FFN) is used. With the EKF approach, the training of the FFN can be seen as state estimation for a non-linear stationary process. The EKF method gives excellent convergence performances provided that there is enough computer core memory and that the machine precision is high. Neural networks are ideally suited to describe the spatial and temporal dependence of tracer-tracer correlations. The neural network performs well even in regions where the correlations are less compact and normally a family of correlation curves would be required. For example, the CH_4-N_2O correlation can be well described using a neural network trained with the latitude, pressure, time of year, and CH_4 volume mixing ratio (v.m.r.). The neural network was able to reproduce the CH_4-N_2O correlation with a correlation coefficient between simulated and training values of 0.9997. The neural network Fortran code used is available for download.

1. Introduction

Compact correlations between long-lived species are well-observed features in the middle atmosphere, as for example described by Fahey et al. (1989); Plumb and Ko (1992); Loewenstein et al. (1993); Elkins et al. (1996); Keim et al. (1997); Michelson et al. (1998); Rinsland et al. (1999); Strahan (1999); Fischer et al. (2000); Muscari et al. (2003). The correlations exist for all long-lived tracers – not just those which are chemically related. This is due to their all be transported by the general circulation of the atmosphere. The tight relationships between different constituents have led to many analyses where measurements of one tracer are used to infer the abundance of another tracer. These correlations can also be used as a diagnostic of mixing (Schoeberl et al., 1997; Morgenstern et al., 2002) and to distinguish between air-parcels of different origins (Waugh and Funatsu, 2003). The description of such spatially and temporally

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dependent correlations are usually achieved by a family of correlations. However, a single neural network is a natural and effective alternative as shown by our previous study (Lary et al., 2004).

This study uses the same dataset as Lary et al. (2004) but uses a quicker and more accurate extended Kalman filter learning algorithm for feed-forward neural networks as described in the next section.

2. Extended Kalman filter as a learning algorithm for feed-forward neural network

For a general introduction to neural networks please see the book by Bishop (1996). In this study we use a new advanced extended Kalman filter learning algorithm for feed-forward neural network. The algorithm used here gave better results in just 3 training epochs (iterations) than our previous study (Lary et al., 2004) using the "JETNET 3.4" package (Lonnblad et al., 1992; Peterson et al., 1994) achieved in 1 million epochs.

It is well known now that finding the optimal synaptic weights of feed-forward neural networks (FNN) employing gradient descent optimization techniques is plagued by extraordinarily slow convergence rates and misfittings (Shah et al., 1992; Blank and Brown, 1994). A number of faster and more accurate methods have been suggested (Blank and Brown, 1994; Iiguni et al., 1992; Watrous, 1987) at the expense of higher computational cost at each iteration. The extended Kalman filter (EKF) is the best known among them (Singhal and Wu, 1989).

With the EKF approach, the training of the FFN can be seen as state estimation for a non-linear stationary process (Singhal and Wu, 1989). What this means exactly will be explained in details in the following sections. The EKF method gives excellent convergence performances provided that there is enough computer core memory and that the machine precision is high. For a large FNN, the storage requirement can become prohibitive. Furthermore, it was noticed (Bierman, 1977) that round off errors due to poor computer precision can sometimes make the algorithm numerically unstable.

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The storage issue has been addressed by a number of research groups (Shah et al., 1992; Puskorius and Feldkamp, 1994). They attacked the estimation problem (training) by partitioning it into a set of subproblems assuming the existence of mutually independent groups of weights; the numerical stability issue can be overcome by using the square root of the estimate error covariance matrix (background error covariance matrix) instead of propagating the full estimate error covariance matrix (Bierman, 1977; Zhang and Li, 1999). It should be, however, noted that only the global (full) EKF is described by Bierman (1977); Zhang and Li (1999). We are not aware of anyone who has combined the partitioning approach with the square root scheme. As our work required neural networks of moderate sizes, we employed the global EKF in conjunction with the square root scheme for training the FNN.

In the following section we describe briefly how the EKF can be used as a training technique for the FNN. We also give a comprehensive description of how our training algorithm has been implemented.

2.1. Employment of EKF As FNN training algorithm

Singhal and Wu (1989) first suggested to use an extended Kalman filter for training neural networks. Their argument was simple and it can be put as follows

- Multilayer feed-forward neural networks can be viewed as a static non-linear dynamic system whose state is the vector containing all its synaptic weights.
- Therefore the training of the neural networks can be considered as a state estimation problem for a stationary non-linear system.
- Furthermore, Kalman filter is known to give an optimal estimate of states of linear dynamic systems. It is also equally well known that an extended version of the Kalman algorithm can be used for estimating the approximate conditional means and covariance of[1] of the non-linear dynamic systems.

[1] conditional mean and covariance: because the EKF is not an optimal filter.

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– Hence, if the neural network is formulated in terms of space-state concepts similar to those of a static non-linear dynamic system, then the best conditional mean and covariance of the synaptic weight vector can be found by employing an extended Kalman filter.

In state estimation form, mathematically the neural network can be described by these two equations (Shah et al., 1992; Zhang and Li, 1999; Haykin, 2001).

$$\mathbf{w}_{j+1} = \mathbf{w}_j + \mathbf{e_j} \quad (1)$$

$$\mathbf{d}_j = \mathbf{h}[\mathbf{w}_j, \mathbf{x}_j] + v_j \quad (2)$$

The first equation is known as the process equation, whereas the second equation is called the observation equation.

– j is the iterative index.

– $\mathbf{h}[\mathbf{w}_j, \mathbf{x}_j]$ is the iterative varying function describing the network; the value of the function is the FNN output.

– $\mathbf{d}_j$ is the known output (observed, desired, or target) vector.

– v_j is the measurement noise vector.

– $\mathbf{x}_j$ is the input vector.

– $\mathbf{w}_j$ is the state (vector elements of which are the synaptic weights) of FNN at j.

– $\mathbf{e}_j$ is the process noise vector.

The assumptions made are:
v_j is a white noise with $E[v_i v_j^T] = \delta_{ij}\mathbf{R}_j$ covariance matrix.
$\mathbf{e}_j$ is a white noise with $E[\mathbf{e}_i \mathbf{e}_j^T] = \delta_{ij}\mathbf{Q}_j$ covariance matrix.
$E[\mathbf{e}_i v_j^T] = 0.$, for all i,j.

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2.2. Training procedure using EKF

The training (state estimation) is now a problem of determining $\hat{\mathbf{w}}$ (the state vector) that minimizes the sum of squared prediction errors of all observed data so far.

Given $\mathbf{d}_j$,$\mathbf{h}_j$,$\mathbf{R}_j$, and $\mathbf{Q}_j$, the EKF solution to finding $\hat{\mathbf{w}}$ can be obtained by using the following recursion (Haykin, 2001)

$$\hat{\mathbf{w}}_j = \hat{\mathbf{w}}_{j-1} + \mathbf{K}_j(\mathbf{d}_j - \hat{\mathbf{y}}_j) \tag{3}$$

$$\mathbf{K}_j = \frac{\mathbf{P}_{j-1}\mathbf{H}_j}{\mathbf{R}_j + \mathbf{H}_j^T\mathbf{P}_{j-1}\mathbf{H}_j} \tag{4}$$

$$\mathbf{P}_j = \mathbf{P}_{j-1} - \mathbf{K}_j\mathbf{H}_j^T\mathbf{P}_{j-1} + \mathbf{Q}_j \tag{5}$$

$\mathbf{K}_j$ is the Kalman gain matrix at step j ; $\mathbf{d}_j - \hat{\mathbf{y}}_j$ vector contains the prediction errors (innovations); $\hat{\mathbf{y}}_j$ is the prediction (=$\mathbf{h}[\mathbf{w}_{j-1}, \mathbf{x}_j]$); $\mathbf{P}_j$ is the estimate of conditional mean covariance matrix; $\mathbf{H}_j$ is a matrix of derivatives of $\mathbf{h}_j$ with respect to all elements of $\hat{\mathbf{w}}_{j-1}$

$$\mathbf{H}_j = \frac{\partial \mathbf{h}[\hat{\mathbf{w}}_{j-1}, \mathbf{x}_j]}{\partial \hat{\mathbf{w}}_{j-1}} \tag{6}$$

2.3. Computational aspects

Consider a neural network with an architecture with one input layer containing n nodes plus one offset node, one hidden layer with m number of nodes plus one offset node, and l number of output nodes in the output layer.

In this architecture $\mathbf{w}$ is a $[m(n+1)+\ m+1]\times l$ vector ; $\mathbf{x}$ is $(n+1)$ where $\mathbf{x}(1)$ is a constant ; $\mathbf{P}$ and $\mathbf{Q}$ are $l[m(n+1)+\ m+1]\times\ l[m(n+1)+\ m+1]$; $\mathbf{R}$ and $\mathbf{d}_j$ are $l\times l$; $\mathbf{K}$ is $[m(n+1)+\ m+1]\times l$; $\mathbf{H}$ is $l[m(n+1)+\ m+1]\times l[m(n+1)+\ m+1]$.

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For the training procedure to work, it requires values of $\mathbf{P}_j$, $\mathbf{R}_j$, and $\mathbf{Q}_j$. $\mathbf{R}_j$ is just the error covariance of the observation (the known data) so it is easy to calculate. $\mathbf{Q}_j$ is usually set to zero. However, $\mathbf{P}$ is not known a priori. So it is initialized at the beginning of the training. Also $\mathbf{w}$ is initialized.

The training procedure is implemented as follows

1. Initializations
   - Choose random values for $\mathbf{w}_0$
   - Set the offsets (biases) to nonzero constants.
   - Initialise $\mathbf{P}_0$ to a small nonzero number.
2. Choose an input training pattern, $\mathbf{x}_j$, which is propagated through the network to yield an output.
3. $\mathbf{R}_j$
   - If the errors of the input pattern are known, calculate $\mathbf{R}_j$.
   - If not, use iteration-varying forgetting factor in its place (Zhang and Li, 1999).
4. Compute $\mathbf{H}_j$
5. Calculate $\mathbf{K}_j$
6. Update
   - $\hat{\mathbf{w}}_j$ by using the Kalman matrix and the innovations.
   - $\mathbf{P}_j$ as shown in Eq. (5).
7. If the stopping criteria is met, exit. Otherwise go back to step 2.

For full details of the process see Sect. 2 in Haykin (2001). In this work:

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– The FNN had only one output, i.e. $\mathbf{d}_j$, $\mathbf{R}_j$, the innovation and the denominator in Eq. (3) are all scalars.

– $\hat{\mathbf{y}}_j = \mathbf{h}(\mathbf{w}, \mathbf{x}) = \tanh[\mathbf{w}(m(n+1)+1 : m+1)^T \mathbf{z}(1 : m+1)]$, where $\mathbf{z}(2 : m+1) = \tanh[\mathbf{w}(1 : n+1)^T \mathbf{x}(1 : n+1)]$ and $\mathbf{x}(1)$ and $\mathbf{z}(1)$ are the biases in the input and hidden layers respectively

– $\mathbf{Q}_j = 0.0$

– $\mathbf{R}_j = I\lambda_j$, where λ_j is a forgetting factor given by Zhang and Li (1999):

$$\lambda_j = \lambda^0 \lambda_{j-1} + (1 - \lambda^0) \tag{7}$$

λ^0 and λ_0 are tunable parameters.

– The square root of $\mathbf{P}$ was initialised and then propagated. This was done to guarantee the numerical stability of the algorithm Bierman (1977).

3. Results: the CH_4-N_2O correlation

Figure 1a shows an example of using the new EKF learning algorithm for feed-forward neural networks for the CH_4-N_2O correlation from the Cambridge 2D model (Law and Pyle, 1993a,b) (red crosses with validation points as green crosses). The CH_4-N_2O data is shown by the yellow filled blue circles. The correlation coefficient between the actual solution and the neural network solution was 0.9997 after just 200 iterations (epochs). The same correlation coefficient is obtained after just 3 iterations (epochs). Overlaid on the same panel are the previous results of Lary et al. (2004) (cyan crosses) which used "Quickprop" learning and required 10^6 iterations to reproduce the CH_4-N_2O correlation with a correlation coefficient between simulated and training values of 0.9995. So the new algorithm gives better results with much less expense. Figure 1b

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shows a scatter diagram of the known N_2O concentration against the neural network N_2O concentration. Figure 1c shows the way the rms error changes with epoch.

Both CH_4 and pressure are strongly correlated with N_2O as can be seen in Fig. 1 of Lary et al. (2004). Latitude and time are only weakly correlated with N_2O but still play a small role in capturing some of the details of the CH_4-N_2O correlation in Panel (a).

A polynomial or other fit will typically do a good job of describing the CH_4-N_2O correlation for high values of CH_4 and N_2O. However, for low values of CH_4 and N_2O there is quite a spread in the relationship which a single curve can not describe. This is the altitude dependent regime where the correlation shows significant variation with altitude (Minschwaner et al., 1996). Figure 1a shows a more conventional fit using a Chebyshev polynomial of order 20 overlaid on the neural network fits. This fit was chosen as giving the best agreement to the CH_4-N_2O correlation after performing fits using 3667 different equations. Even though this is a good fit the spread of values can not be described by a single curve. However, a neural network trained with the latitude, pressure, time of year, and CH_4 volume mixing ratio (v.m.r.) (four inputs) is able to well reproduce the N_2O v.m.r. (one output), including the spread for low values of CH_4 and N_2O.

3.1. Scaling

Variable scaling often allows neural networks to achieve better results. In this case all variables were scaled to vary between ±1. If the initial range of values was more than an order of magnitude then log scaling was also applied. In the case of time of year the sine of the fractional time of year was used to avoid a step discontinuity at the start of the year.

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4. Conclusions

Neural networks are ideally suited to describe the spatial and temporal dependence of tracer-tracer correlations. Even in regions when the correlations are less compact. Using a new extended Kalman filter learning algorithm for feed-forward neural networks the correlation coefficient between the actual solution and the neural network solution was 0.9997 after just 200 iterations (epochs). The same correlation coefficient is obtained after just 3 iterations (epochs). This can be compared to our previous study (Lary et al., 2004) which used "Quickprop" learning and required 10^6 iterations to reproduce the CH_4-N_2O correlation with a correlation coefficient between simulated and training values of 0.9995. So the new algorithm gives better results with much less expense.

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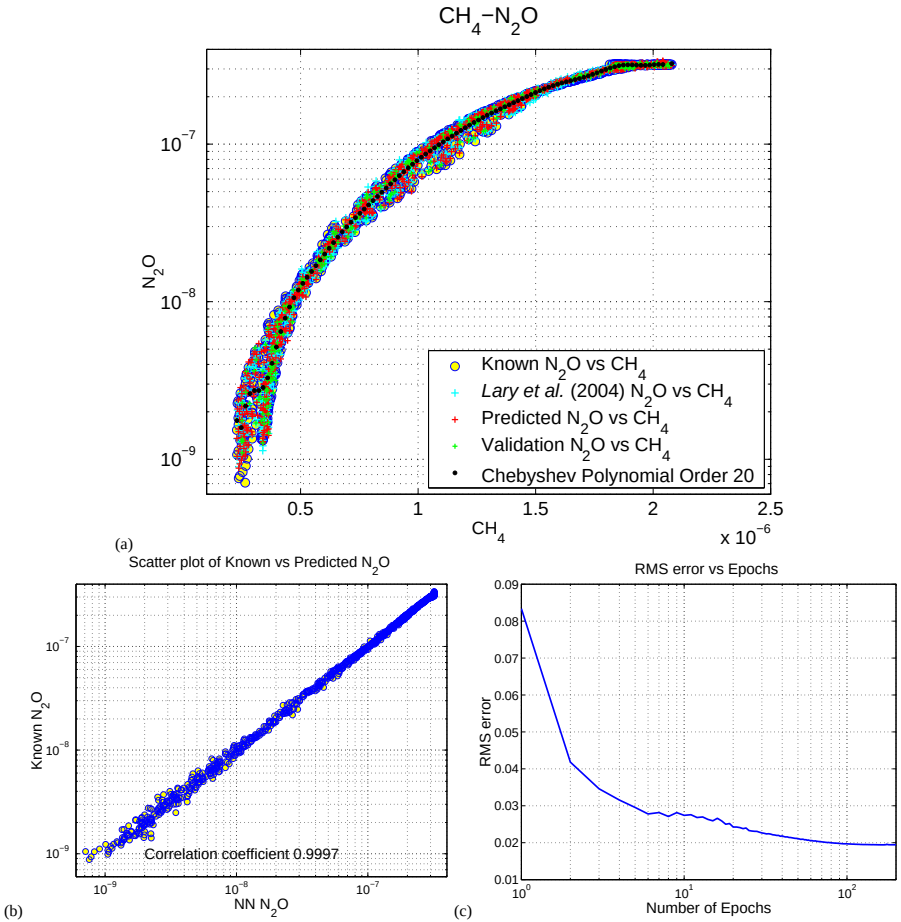

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Neural networks and tracer correlations

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Fig. 1. The neural network used to produce the CH_4-N_2O correlation in **(a)** is our new extended Kalman filter learning algorithm for feed-forward neural networks (red crosses with validation points as green crosses). The data is shown by the yellow filled blue circles. The correlation coefficient between the actual solution and the neural network solution was 0.9997 after just 200 iterations (epochs). The same correlation coefficient is obtained after just 3 iterations (epochs). Overlaid on the same panel are the previous results of Lary et al. (2004) (cyan crosses) which used "Quickprop" learning and required 10^6 iterations to reproduce the CH_4-N_2O correlation with a correlation coefficient between simulated and training values of 0.9995. A Chebyshev polynomial of order 20 is also shown (small black circles) for the sake of comparison. This fit was chosen as giving the best agreement to the CH_4-N_2O correlation after performing fits using 3667 different equations. Even though this is a good fit the spread of values can not be described by a single curve. However, a neural network trained with the latitude, pressure, time of year, and CH_4 volume mixing ratio (v.m.r.) (four inputs) is able to well reproduce the N_2O v.m.r. (one output), including the spread for low values of CH_4 and N_2O. **(b)** shows a scatter diagram of the known N_2O concentration against the neural network N_2O concentration. **(c)** shows the way the rms error changes with epoch.

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