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SUPPLEMENTARY MATERIAL TO Modeling of methane emissions using the artificial neural network approach

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DETAILS OF ANN ARCHITECTURES

BPNN is a three-layer feed-forward network trained from input data using an error backpropagation algorithm. This is a supervised network, *i.e.*, trained with both inputs and outputs. A three-layer BPNN network with standard connections is suitable for almost all problems of this nature.¹ The learning process of a BP network consists of two iterative steps: forward computing of the data stream and backward propagation of error signals. During the forward computing, the original data are transmitted from the input layer to the output layer through the hidden processing layer and the neurons of each layer can only affect the neurons of the next layer. In this process, the synaptic weights are all adjusted in accordance with the error signals. With these two steps being performed iteratively, the error, *i.e.*, the difference between the network output and desired output, can be minimized using the delta rule.²

The number of neurons in the input and output layer is equal to the number of input and output parameters that are used in the BPNN model, while the number of neurons in the hidden layer is often computed as the sum of half of the inputs plus the output neurons and the square root of the number of training patterns. The number of neurons in the hidden layer in the employed BPNN model was 15, the logistic activation function was used, and the learning rate and momentum parameters were set to a value of 0.1. The training time was 30 min during which 73952 learning epochs were performed. The schematic representation of the BPNN model is presented in Fig. 1a.

A GRNN is also a feed forward neural network with supervised training based on the nonlinear regression theory. It consists of an input layer, a hidden layer that can be divided into a pattern layer and a summation layer and an output layer. GRNNs work by measuring how far a given sample pattern is from the patterns in the training set in N-dimensional space, where Nis the number of inputs in the problem. The training of the GRNN is quite different from the training used in BP neural networks, being completed after presentation of each input–output vector pair from the training data set to the GRNN input layer only once. The resulting parameter of the GRNN training is a smoothing factor, which determines how tightly the

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network matches its predictions to the data in the training patterns.¹ The number of neurons in the input and output layer is equal to the number of input and output parameters that were used in the ANN model. The number of neurons in the pattern sub-layer is equal to the number of training cases used for model training, *i.e.*, 160 neurons. The input data was scaled using a linear function in range of 0 to 1, and the smoothing factor was determined using a genetic algorithm.³ The schematic representation of the GRNN is shown in Fig. 1b.



Fig. S-1. Schemas of the used ANN architectures: a) BPNN and b) GRNN.

For neural network design and training, the software tool NeuroShell 2 was used.⁴

TRAINING AND TEST DATA SETS

Country	GDP	WDL	MWG	NC	<i>LR</i> ×10 ⁻⁷	PPG	CH ₄ emission
		kg pc	kg pc	cattle pc	ha pc	toe pc	kg pc
Bulgaria	0.14	357	461	0.082	5.83	0.048	78.05
Czech Republic	0.49	199	296	0.136	0	0.014	55.77
Denmark	1.70	37	740	0.291	0	1.718	68.83
Estonia	0.42	278	399	0.182	0	0.000	78.68
Greece	0.79	385	442	0.061	20.8	0.002	35.41
Spain	0.95	355	594	0.141	24.3	0.001	39.25
France	1.20	194	536	0.299	27.4	0.017	62.68
Latvia	0.30	293	412	0.164	0	0.000	65.68
Lithuania	0.30	357	391	0.246	0	0.000	71.30
Luxembourg	3.03	130	683	0.397	0	0.000	108.65
Hungary	0.38	376	468	0.070	2.38	0.236	36.81
Netherlands	1.40	15	622	0.225	0	3.391	60.85

TABLE S-I. Training dataset for the year 2006

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Country		WDL	MWG	NC	<i>LR</i> ×10 ⁻⁷	PPG	CH ₄ emission
	GDF	kg pc	kg pc	cattle pc	ha pc	toe pc	kg pc
Austria	1.32	25	653	0.243	0	0.189	48.64
Poland	0.30	236	321	0.138	0	0.102	87.27
Portugal	0.64	297	463	0.133	24.0	0.000	58.38
Romania	0.19	292	389	0.136	2.59	0.442	58.41
Slovenia	0.65	361	431	0.227	0	0.001	70.65
Slovakia	0.35	234	301	0.094	0	0.033	36.12
Finland	1.33	286	494	0.177	0	0.000	88.82
UK	1.36	352	586	0.171	0	1.192	49.67

TABLE S-I. Continued

TABLE S-II. Test data set

Country	GDP	WDL	MWG	NC	$LR \times 10^{-7}$	PPG
Country		kg pc	kg pc	cattle pc	ha pc	toe pc
Bulgaria	0.16	389	433	0.080	8.59	0.031
Czech Republic	0.51	205	293	0.133	0	0.016
Denmark	1.67	37	790	0.284	0	1.518
Estonia	0.48	291	449	0.179	0	0.000
Greece	0.80	357	447	0.061	23	0.002
Spain	0.94	347	583	0.148	21.6	0.000
France	1.18	194	543	0.300	2.59	0.014
Latvia	0.37	323	378	0.175	0	0.000
Lithuania	0.34	369	401	0.233	0	0.000
Luxembourg	3.12	126	695	0.406	0	0.000
Hungary	0.40	341	457	0.070	2.58	0.199
Netherlands	1.40	13	629	0.234	0	3.328
Austria	1.32	20	596	0.241	0	0.192
Poland	0.33	239	322	0.142	0	0.102
Portugal	0.64	299	468	0.136	25.4	0.000
Romania	0.23	284	379	0.131	3.9	0.428
Slovenia	0.68	341	439	0.239	0	0.001
Slovakia	0.41	240	309	0.093	0	0.020
Finland	1.36	267	506	0.171	0	0.000
UK	1.35	323	570	0.166	0	1.068
Bulgaria	0.18	441	474	0.075	10.2	0.020
Czech Rep.	0.59	197	305	0.131	0	0.016
Denmark	1.71	32	830	0.292	0	1.646
Estonia	0.49	248	391	0.177	0	0.000
Greece	0.83	372	452	0.061	24.1	0.001
Spain	0.96	287	556	0.133	21.1	0.000
France	1.20	171	541	0.303	2.56	0.013
Latvia	0.40	311	332	0.167	0	0.000
Lithuania	0.39	368	408	0.229	0	0.000
Luxembourg	3.23	123	697	0.406	0	0.000
Hungary	0.42	333	454	0.070	2.49	0.200
Netherlands	1.45	8	624	0.244	0	3.651

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TABLE S	-II. Continue	d
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Country	GDP	WDL	MWG	NC	LR×10 ⁻⁷	PPG
		kg pc	kg pc	cattle pc	ha pc	toe pc
Austria	1.36	19	599	0.240	0	0.158
Poland	0.38	228	320	0.146	0	0.097
Portugal	0.65	332	515	0.136	24.8	0.000
Romania	0.26	301	392	0.125	4.6	0.418
Slovenia	0.74	339	457	0.234	0	0.001
Slovakia	0.48	250	328	0.090	0	0.016
Finland	1.40	265	521	0.171	0	0.000
UK	1.17	287	544	0.162	0	1.025

REFERENCES

1. S. A. Kalogirou, Prog. Energ. Combust. 29 (2003) 515

 M. Cai, Y. Yin, M. Xie, *Transport Res. D-TrE* 14 (2009) 32.
Neuroshell 2 Help, GRNN Training Criteria, Ward Systems Group Inc., http:// //www.wardsystems.com/manuals/neuroshell2/index.html?idxhowuse.htm (Accessed 20 August 2014)

4. Neuroshell 2, Ward Systems Group Inc., Frederick, MD, 1993.