Poster presentation at 2nd European User Meeting on Multivariate Analysis
Como, Italy, 21 - 23 June 2006

Prediction of Oxygen-18 Concentrations in Precipitation

A. Liebminger[1], G. Heiss[1], W. Papesch[1],
G. Haberhauer[1] and K. Varmuza[2]*

[1] Biogenetics - Natural Resources, Austrian Research Centers Seibersdorf, A-2444 Seibersdorf, Austria, seibersdorf@arcs.ac.at

[2] Laboratory for Chemometrics, Institute of Chemical Engineering, Vienna University of Technology, Getreidemarkt 9/166, A-1060 Vienna, Austria, kvarmuza@email.tuwien.ac.at

seibersdorf research
An Enterprise of the Austrian Research Centers.

TU WIEN

LCM

www.lcm.tuwien.ac.at

Introduction

Stable isotope data of precipitation are recognized as a major reference for many hydrological applications. Oxygen-18 records of precipitation have been used to validate atmospheric global circulation models and to calibrate isotope records in paleoclimatic archives, such as ice cores, lake sediments, tree rings and groundwater.

Aim of this study was modeling O-18 concentrations in precipitation by meteorological and geographical features.

Isotope ratio mass spectrometry data obtained from 5000 precipitation samples, collected at 30 locations in Austria, have been selected from the database *Austrian Network of Isotopes in Precipitation* (*ANIP*). Each location has been characterized by the long term monthly means of O-18 concentrations, five meteorological parameters, and the three geographical attributes longitude, latitude and elevation of the sampling station. This basic feature set has been augmented by nonlinear transformations and cross terms of the original features [1].

The O-18 values are reported in δ - notation as per mill (‰) relative to the V-SMOW (Vienna Standard Mean Ocean Water) standard.

Initial Situation

For locations with no data available the δ O-18 values can be estimated by interpolation of data from neighboring stations (Fig. 1). However, this approach is insufficient because interpolation does not consider geographic parameters like latitude and altitude.

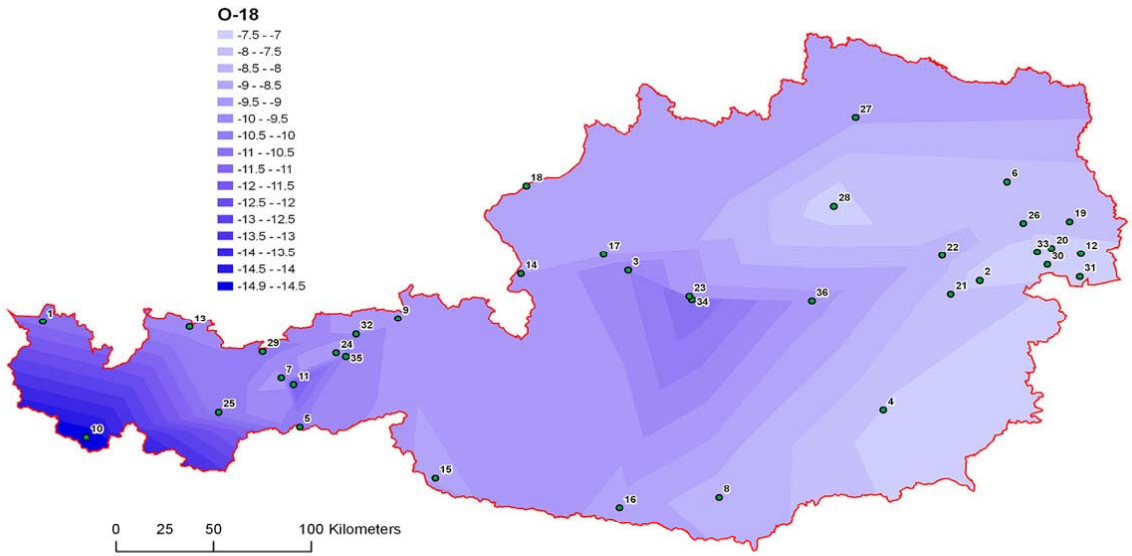

Fig.1: δ O-18 values in precipitation: Interpolation with experimental data from 36 sampling stations.

Results and Discussion

A set of 102 cases has been used as calibration set and 78 other cases as application set, with each case representing data at a sampling site for one month from the summer half year. Regression models have been developed by the methods OLS and PLS.

Different methods of feature selection have been applied (Tab. 1). A new method for feature selection (FASS) is based on a combination of stepwise forward selection and all subsets regression [2].

Geographical isotope distribution maps of O-18 values, created from predicted data, lead to more reasonable O-18 distributions (Fig. 2) than maps computed only from experimental data of 36 sampling locations (Fig. 1).

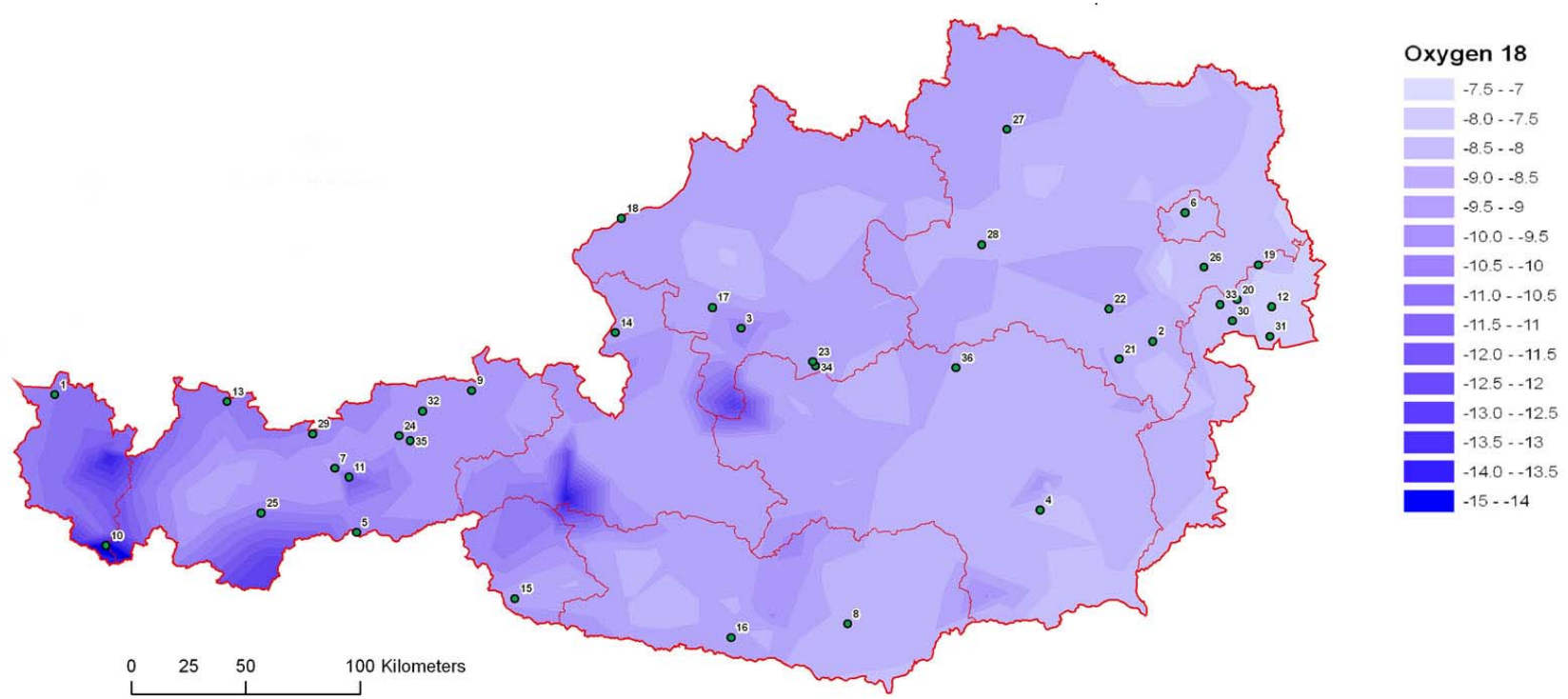

Fig. 2: δ O-18 values in precipitation: Interpolation with modeled data from 201 stations with meteorological values available. The SEP between the experimental data of the 36 sample stations and the map values is 0.59 per mill.

Tab. 1: Summary of best results for various feature selection methods.

	All feature set	Feature selection by PLS regr coeff.	Stepwise feature selection*	GA feature selection	FASS feature selection	FASS feature selection
p	57	25	23	11	13	15
a_{PLS}	18	21	19	11	13	14
R^2_{CV}	0.8457	0.8594	0.9086	0.9046	0.9066	0.9145
${}_{ADJ}R^2_{CV}$	0.6537	0.8156	0.8831	0.8941	0.8940	0.9008
SEP_{CV}	0.93	0.88	0.71	0.73	0.72	0.69
R^2_{APPL}	0.6206	0.2467	0.6598	0.7736	0.7677	0.7052
${}_{ADJ}R^2_{APPL}$	0.1485	0.0118	0.5651	0.7430	0.7364	0.6576
SEP_{APPL}	1.17	1.59	1.06	0.90	0.90	1.00

Regression model for O-18 values in precipitation

$$\delta^{18}O = 5.99 + 0.874\,t - 0.186\,p - 0.00814\,h.t + 0.00151\,h.p + 0.000393\,e.t + 0.0000308\,e.s + 0.00793\,p.w + 0.00272\,l.p - 0.114\,l.w + 0.000293\,e.l + 0.201\,w^2 - 0.00000172\,e^2 - 3.04 \log e$$

t	temperature [°C]
p	amount of precipitation [mm]
h	relative humidity [%]
e	elevation [m above sea level]
w	wind speed [ms^{-1}]
l	longitude [dec.°]
s	fresh snow amount [mm]

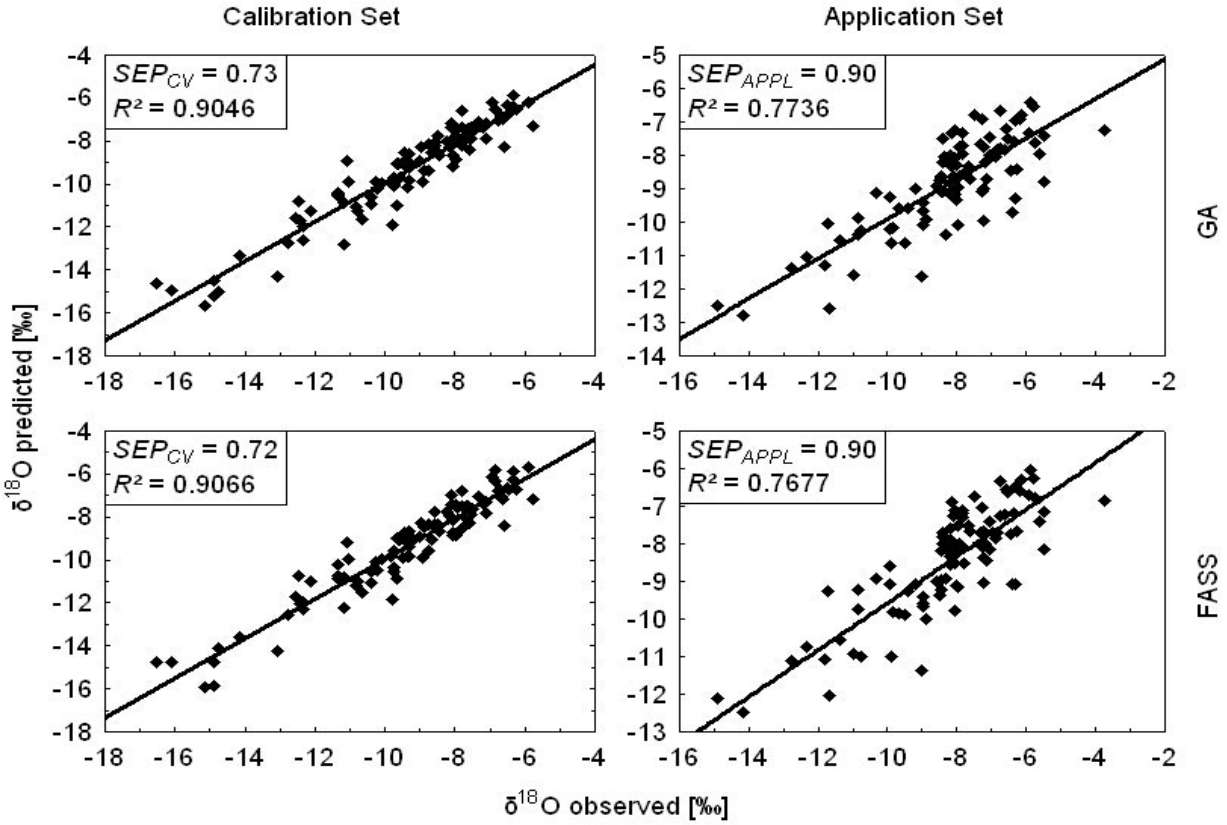

Fig. 3: Predicted versus observed δ O-18 values for the best model obtained by FASS features selection (second row) in comparison with the best model obtained by GA feature selection (first row). Predicted values for the calibration set are from leave-one-out cross validation.

References

[1] Liebminger A., Haberhauer G., Papesch W. and Heiss G., Correlation of the isotopic Composition in Precipitation with local Conditions in Alpine Regions, J. Geophys. Res. 111 (2006) L05808..

[2] Liebminger A., Dissertation, Vienna University of Technology (2006).